(dme)$TaCl_3(NNPh_2)$: A Versatile Synthon for Terminal Hydrazido(2-) Tantalum Complexes

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Supporting Information

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CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 6 February 2009

Crystal Structure Analysis of:

Complex 1 (IAT31)

(shown below)

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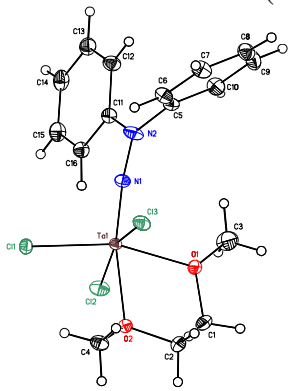


IAT31

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC). The deposition number is 719414.

Table 1. Crystal data and structure refinement for IAT31 (CCDC 719414).

Empirical formula	$C_{16}H_{20}N_2O_2Cl_3Ta$
Formula weight	559.64
Crystallization Solvent	Dichloroethane/Pentane
Crystal Habit	Purple
Crystal size	0.21 x 0.08 x 0.07 mm^3
Crystal color	Needle

Data Collection

Type of diffractometer	Bruker KAPPA APEX II	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 9998 reflections used in lattice determination	2.67 to 52.01°	
Unit cell dimensions	a = 13.4839(6) Å b = 10.2768(4) Å c = 14.8254(7) Å	β= 108.079(2)°
Volume	1952.95(15) $Å^3$	
Z	4	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Density (calculated)	1.903 Mg/m^3	
F(000)	1080	
Data collection program	Bruker APEX2 v2.1-0	
θ range for data collection	1.59 to 52.22°	
Completeness to θ = 52.22°	94.5 %	
Index ranges	$-27 \le h \le 29$, $-21 \le k \le 22$, $-22 \le l \le 31$	
Data collection scan type	ω scans; 22 settings	
Data reduction program	Bruker SAINT-Plus v7.34A	
Reflections collected	116353	
Independent reflections	21254 [R_{int}= 0.0360]	
Absorption coefficient	6.049 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7503 and 0.5013	

Table 1 (cont.)

Structure solution and Refinement

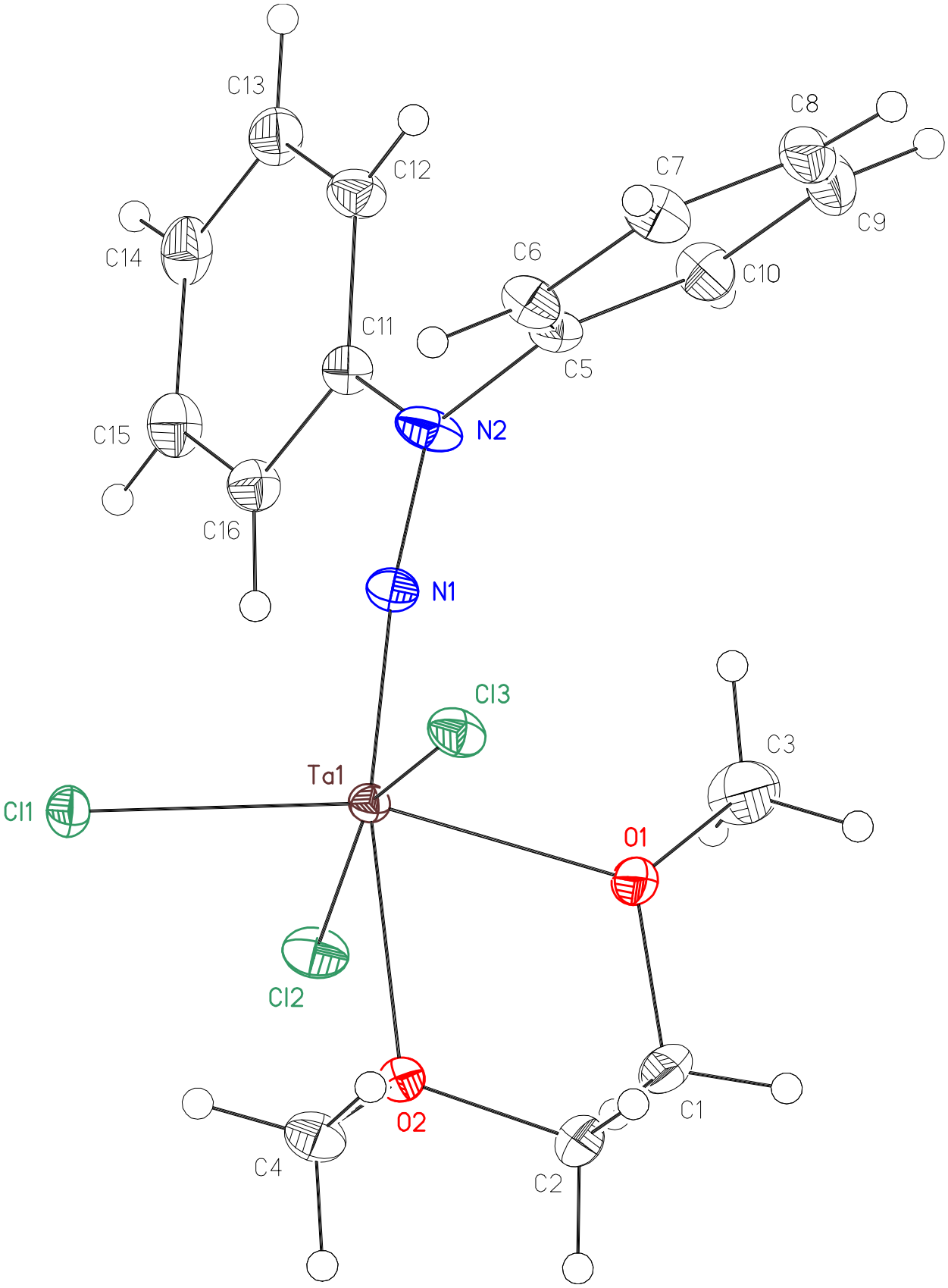
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	21254 / 0 / 297
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.388
Final R indices [$I>2\sigma(I)$, 16090 reflections]	R1 = 0.0285, *w*R2 = 0.0362
R indices (all data)	R1 = 0.0513, *w*R2 = 0.0380
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.008
Average shift/error	0.000
Largest diff. peak and hole	4.620 and -2.759 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C11
C15
C16
N2
N1
C8
C7
C9
C6
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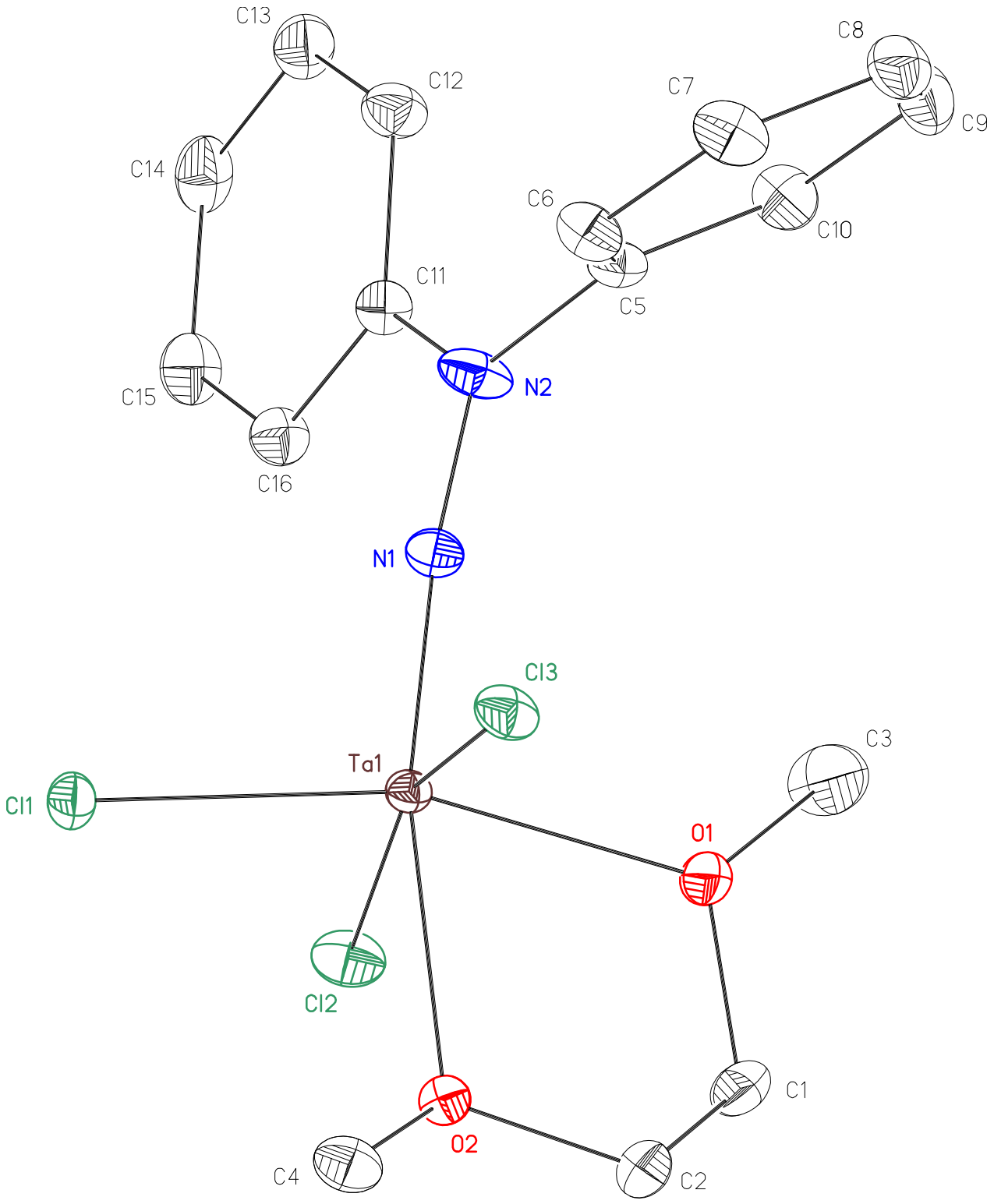
Cl1
C3
O1
Cl2
O2
C1
C4
C2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C12
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C11
C15
C16
N2
N1
C8
C7
C9
C6
C10
C5
Cl3
Ta1
Cl1
C3
O1
Cl2
C1
O2
C4
C2

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT31 (CCDC 719414). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	1522(1)	7414(1)	4494(1)	10(1)
Cl(1)	729(1)	5852(1)	3314(1)	15(1)
Cl(2)	2644(1)	5763(1)	5431(1)	19(1)
Cl(3)	191(1)	8997(1)	3912(1)	17(1)
O(1)	2015(1)	8477(1)	5818(1)	19(1)
O(2)	427(1)	6815(1)	5336(1)	14(1)
N(1)	2439(1)	8147(1)	4015(1)	14(1)
N(2)	3131(1)	8820(1)	3711(1)	18(1)
C(1)	1694(1)	7913(1)	6588(1)	24(1)
C(2)	560(1)	7583(1)	6185(1)	20(1)
C(3)	3031(2)	9094(2)	6175(1)	44(1)
C(4)	-671(1)	6538(1)	4882(1)	19(1)
C(5)	2968(1)	10198(1)	3602(1)	14(1)
C(6)	2019(1)	10663(1)	3018(1)	17(1)
C(7)	1839(1)	11996(1)	2942(1)	21(1)
C(8)	2600(1)	12860(1)	3443(1)	21(1)
C(9)	3550(1)	12389(1)	4018(1)	23(1)
C(10)	3737(1)	11059(1)	4101(1)	20(1)
C(11)	3980(1)	8160(1)	3558(1)	14(1)
C(12)	4587(1)	8777(1)	3072(1)	19(1)
C(13)	5422(1)	8120(1)	2923(1)	21(1)
C(14)	5669(1)	6861(1)	3249(1)	21(1)
C(15)	5047(1)	6242(1)	3712(1)	20(1)
C(16)	4207(1)	6878(1)	3869(1)	16(1)

Table 3. Selected bond lengths [Å] and angles [°] for IAT31 (CCDC 719414).

Ta(1)-N(1)	1.7727(8)	N(1)-Ta(1)-O(1)	95.34(3)
Ta(1)-O(1)	2.1638(7)	N(1)-Ta(1)-O(2)	168.03(3)
Ta(1)-O(2)	2.2954(7)	O(1)-Ta(1)-O(2)	73.10(3)
Ta(1)-Cl(1)	2.3711(2)	N(1)-Ta(1)-Cl(1)	101.76(3)
Ta(1)-Cl(3)	2.3780(2)	O(1)-Ta(1)-Cl(1)	162.30(2)
Ta(1)-Cl(2)	2.4065(3)	O(2)-Ta(1)-Cl(1)	90.034(19)
		N(1)-Ta(1)-Cl(3)	96.08(3)
		O(1)-Ta(1)-Cl(3)	88.16(2)
		O(2)-Ta(1)-Cl(3)	80.773(19)
		Cl(1)-Ta(1)-Cl(3)	94.507(9)
		N(1)-Ta(1)-Cl(2)	98.01(3)
		O(1)-Ta(1)-Cl(2)	82.61(2)
		O(2)-Ta(1)-Cl(2)	83.81(2)
		Cl(1)-Ta(1)-Cl(2)	90.427(10)
		Cl(3)-Ta(1)-Cl(2)	163.803(9)

Table 4. Bond lengths [Å] and angles [°] for IAT31 (CCDC 719414).

Ta(1)-N(1)	1.7727(8)	O(1)-Ta(1)-Cl(1)	162.30(2)
Ta(1)-O(1)	2.1638(7)	O(2)-Ta(1)-Cl(1)	90.034(19)
Ta(1)-O(2)	2.2954(7)	N(1)-Ta(1)-Cl(3)	96.08(3)
Ta(1)-Cl(1)	2.3711(2)	O(1)-Ta(1)-Cl(3)	88.16(2)
Ta(1)-Cl(3)	2.3780(2)	O(2)-Ta(1)-Cl(3)	80.773(19)
Ta(1)-Cl(2)	2.4065(3)	Cl(1)-Ta(1)-Cl(3)	94.507(9)
O(1)-C(3)	1.4527(17)	N(1)-Ta(1)-Cl(2)	98.01(3)
O(1)-C(1)	1.4597(13)	O(1)-Ta(1)-Cl(2)	82.61(2)
O(2)-C(2)	1.4478(12)	O(2)-Ta(1)-Cl(2)	83.81(2)
O(2)-C(4)	1.4518(14)	Cl(1)-Ta(1)-Cl(2)	90.427(10)
N(1)-N(2)	1.3465(11)	Cl(3)-Ta(1)-Cl(2)	163.803(9)
N(2)-C(11)	1.4084(13)	C(3)-O(1)-C(1)	111.32(9)
N(2)-C(5)	1.4346(12)	C(3)-O(1)-Ta(1)	122.63(8)
C(1)-C(2)	1.4975(18)	C(1)-O(1)-Ta(1)	115.28(6)
C(1)-H(1A)	0.945(14)	C(2)-O(2)-C(4)	110.13(8)
C(1)-H(1B)	0.996(16)	C(2)-O(2)-Ta(1)	113.52(6)
C(2)-H(2A)	0.979(13)	C(4)-O(2)-Ta(1)	122.43(6)
C(2)-H(2B)	0.957(14)	N(2)-N(1)-Ta(1)	173.65(7)
C(3)-H(3A)	0.93(2)	N(1)-N(2)-C(11)	119.29(8)
C(3)-H(3B)	0.985(19)	N(1)-N(2)-C(5)	116.51(8)
C(3)-H(3C)	0.98(3)	C(11)-N(2)-C(5)	124.15(8)
C(4)-H(4A)	0.992(13)	O(1)-C(1)-C(2)	106.92(9)
C(4)-H(4B)	0.939(15)	O(1)-C(1)-H(1A)	108.5(8)
C(4)-H(4C)	0.943(14)	C(2)-C(1)-H(1A)	108.8(9)
C(5)-C(6)	1.3877(15)	O(1)-C(1)-H(1B)	106.6(8)
C(5)-C(10)	1.3891(15)	C(2)-C(1)-H(1B)	113.1(9)
C(6)-C(7)	1.3895(15)	H(1A)-C(1)-H(1B)	112.7(12)
C(6)-H(6)	0.917(15)	O(2)-C(2)-C(1)	107.87(9)
C(7)-C(8)	1.3862(18)	O(2)-C(2)-H(2A)	108.3(8)
C(7)-H(7)	0.890(19)	C(1)-C(2)-H(2A)	109.2(8)
C(8)-C(9)	1.3876(18)	O(2)-C(2)-H(2B)	107.5(8)
C(8)-H(8)	0.863(15)	C(1)-C(2)-H(2B)	113.3(8)
C(9)-C(10)	1.3886(15)	H(2A)-C(2)-H(2B)	110.5(11)
C(9)-H(9)	0.947(17)	O(1)-C(3)-H(3A)	107.2(13)
C(10)-H(10)	0.929(16)	O(1)-C(3)-H(3B)	109.6(11)
C(11)-C(16)	1.3976(14)	H(3A)-C(3)-H(3B)	109.8(16)
C(11)-C(12)	1.3989(14)	O(1)-C(3)-H(3C)	109.8(16)
C(12)-C(13)	1.3880(15)	H(3A)-C(3)-H(3C)	108.3(17)
C(12)-H(12)	0.882(14)	H(3B)-C(3)-H(3C)	112.0(18)
C(13)-C(14)	1.3852(17)	O(2)-C(4)-H(4A)	108.9(9)
C(13)-H(13)	0.931(14)	O(2)-C(4)-H(4B)	108.7(10)
C(14)-C(15)	1.3921(16)	H(4A)-C(4)-H(4B)	109.1(12)
C(14)-H(14)	0.943(14)	O(2)-C(4)-H(4C)	109.6(9)
C(15)-C(16)	1.3880(15)	H(4A)-C(4)-H(4C)	109.6(11)
C(15)-H(15)	0.899(14)	H(4B)-C(4)-H(4C)	110.9(12)
C(16)-H(16)	0.952(14)	C(6)-C(5)-C(10)	120.26(9)
		C(6)-C(5)-N(2)	119.36(9)
N(1)-Ta(1)-O(1)	95.34(3)	C(10)-C(5)-N(2)	120.34(10)
N(1)-Ta(1)-O(2)	168.03(3)	C(5)-C(6)-C(7)	119.65(10)
O(1)-Ta(1)-O(2)	73.10(3)	C(5)-C(6)-H(6)	120.4(9)
N(1)-Ta(1)-Cl(1)	101.76(3)	C(7)-C(6)-H(6)	119.9(9)

C(8)-C(7)-C(6)	120.42(11)	C(13)-C(12)-C(11)	119.65(10)
C(8)-C(7)-H(7)	122.6(11)	C(13)-C(12)-H(12)	120.4(9)
C(6)-C(7)-H(7)	117.0(11)	C(11)-C(12)-H(12)	120.0(9)
C(7)-C(8)-C(9)	119.60(10)	C(14)-C(13)-C(12)	121.18(10)
C(7)-C(8)-H(8)	123.0(10)	C(14)-C(13)-H(13)	120.1(9)
C(9)-C(8)-H(8)	117.2(10)	C(12)-C(13)-H(13)	118.7(9)
C(8)-C(9)-C(10)	120.40(11)	C(13)-C(14)-C(15)	118.84(10)
C(8)-C(9)-H(9)	123.7(10)	C(13)-C(14)-H(14)	123.0(9)
C(10)-C(9)-H(9)	115.9(10)	C(15)-C(14)-H(14)	118.2(9)
C(9)-C(10)-C(5)	119.65(11)	C(16)-C(15)-C(14)	121.04(10)
C(9)-C(10)-H(10)	121.6(10)	C(16)-C(15)-H(15)	120.0(9)
C(5)-C(10)-H(10)	118.8(10)	C(14)-C(15)-H(15)	118.9(9)
C(16)-C(11)-C(12)	119.61(9)	C(15)-C(16)-C(11)	119.65(10)
C(16)-C(11)-N(2)	120.43(9)	C(15)-C(16)-H(16)	121.5(9)
C(12)-C(11)-N(2)	119.95(9)	C(11)-C(16)-H(16)	118.6(9)

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT31 (CCDC 719414). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	109(1)	95(1)	98(1)	11(1)	31(1)	0(1)
Cl(1)	181(1)	138(1)	131(1)	-20(1)	37(1)	-13(1)
Cl(2)	154(1)	191(1)	195(1)	81(1)	29(1)	33(1)
Cl(3)	171(1)	120(1)	217(1)	44(1)	76(1)	36(1)
O(1)	246(4)	209(3)	128(3)	-38(3)	63(3)	-100(3)
O(2)	163(3)	135(3)	138(3)	-3(2)	65(3)	-8(2)
N(1)	130(4)	134(3)	144(3)	29(3)	42(3)	6(3)
N(2)	154(4)	137(3)	295(5)	72(3)	130(4)	30(3)
C(1)	315(7)	278(5)	129(4)	-33(4)	94(4)	-92(5)
C(2)	274(6)	186(4)	187(4)	-35(4)	129(4)	-19(4)
C(3)	468(10)	636(11)	208(6)	-119(7)	83(6)	-407(9)
C(4)	155(5)	199(4)	233(5)	26(4)	77(4)	-18(4)
C(5)	138(4)	135(3)	159(4)	38(3)	66(3)	19(3)
C(6)	129(4)	163(4)	212(5)	32(3)	28(4)	-4(3)
C(7)	155(5)	177(4)	275(5)	64(4)	52(4)	45(3)
C(8)	254(6)	139(4)	264(5)	8(4)	117(5)	27(4)
C(9)	259(6)	183(4)	208(5)	-29(4)	23(4)	-36(4)
C(10)	170(5)	200(4)	181(5)	27(3)	2(4)	2(4)
C(11)	115(4)	152(4)	153(4)	6(3)	40(3)	12(3)
C(12)	174(5)	179(4)	228(5)	18(4)	98(4)	-1(3)
C(13)	174(5)	230(5)	238(5)	-51(4)	104(4)	-31(4)
C(14)	152(5)	230(5)	257(5)	-80(4)	70(4)	8(4)
C(15)	187(5)	176(4)	226(5)	-10(4)	49(4)	46(4)
C(16)	163(5)	156(4)	173(4)	14(3)	50(4)	18(3)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for IAT31 (CCDC 719414).

	x	y	z	U_{iso}
H(1A)	1776(11)	8550(15)	7065(9)	21(4)
H(1B)	2144(13)	7136(15)	6814(10)	24(4)
H(2A)	350(11)	7052(13)	6643(9)	16(3)
H(2B)	121(11)	8332(13)	6009(9)	14(3)
H(3A)	3000(16)	9670(20)	6645(14)	63(6)
H(3B)	3185(15)	9570(20)	5656(13)	59(6)
H(3C)	3560(20)	8440(30)	6460(17)	98(9)
H(4A)	-952(11)	6092(14)	5345(10)	23(4)
H(4B)	-736(13)	5984(15)	4363(10)	30(4)
H(4C)	-1037(12)	7322(13)	4685(10)	15(3)
H(6)	1508(12)	10096(14)	2692(9)	23(4)
H(7)	1214(15)	12255(16)	2575(12)	36(5)
H(8)	2500(11)	13689(14)	3446(9)	21(4)
H(9)	4108(13)	12928(15)	4365(11)	28(4)
H(10)	4365(12)	10725(15)	4490(10)	29(4)
H(12)	4439(11)	9579(14)	2864(9)	21(4)
H(13)	5819(11)	8542(14)	2598(9)	20(4)
H(14)	6248(12)	6404(14)	3179(9)	21(4)
H(15)	5210(11)	5428(14)	3930(9)	22(4)
H(16)	3816(11)	6491(14)	4234(9)	22(4)

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 24 February 2010

Crystal Structure Analysis of:

Complex 7 (IAT49)

(shown below)

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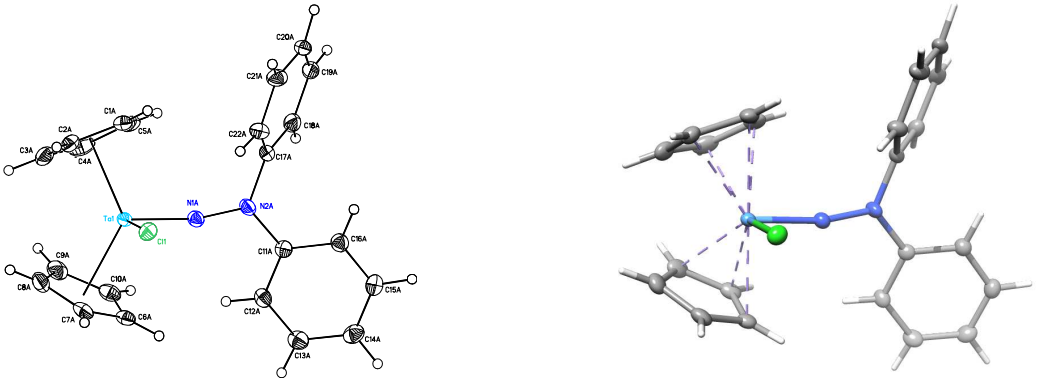
Contents



IAT49

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC). The deposition number is 767430.

Table 1. Crystal data and structure refinement for IAT49 (CCDC 767430).

Empirical formula	$C_{22}H_{20}N_2ClTa$
Formula weight	528.80
Crystallization Solvent	Toluene/pentane @-30ºC
Crystal Habit	Fragment
Crystal size	0.19 x 0.18 x 0.11 mm^3
Crystal color	Orange

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9653 reflections used in lattice determination	2.42 to 39.13°
Unit cell dimensions	a = 19.1261(8) Å b = 10.2503(4) Å β= 100.720(2)° c = 19.2383(8) Å
Volume	3705.8(3) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	P $2_1/n$
Density (calculated)	1.896 Mg/m^3
F(000)	2048
Data collection program	Bruker APEX2 v2009.7-0
θ range for data collection	2.26 to 40.86°
Completeness to θ = 40.86°	95.0 %
Index ranges	$-31 \le h \le 34$, $-18 \le k \le 18$, $-35 \le l \le 22$
Data collection scan type	ω scans; 14 settings
Data reduction program	Bruker SAINT-Plus v7.66A
Reflections collected	148999
Independent reflections	22998 [R_{int}= 0.0412]
Absorption coefficient	6.084 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7481 and 0.5946

Table 1 (cont.)

Structure solution and Refinement

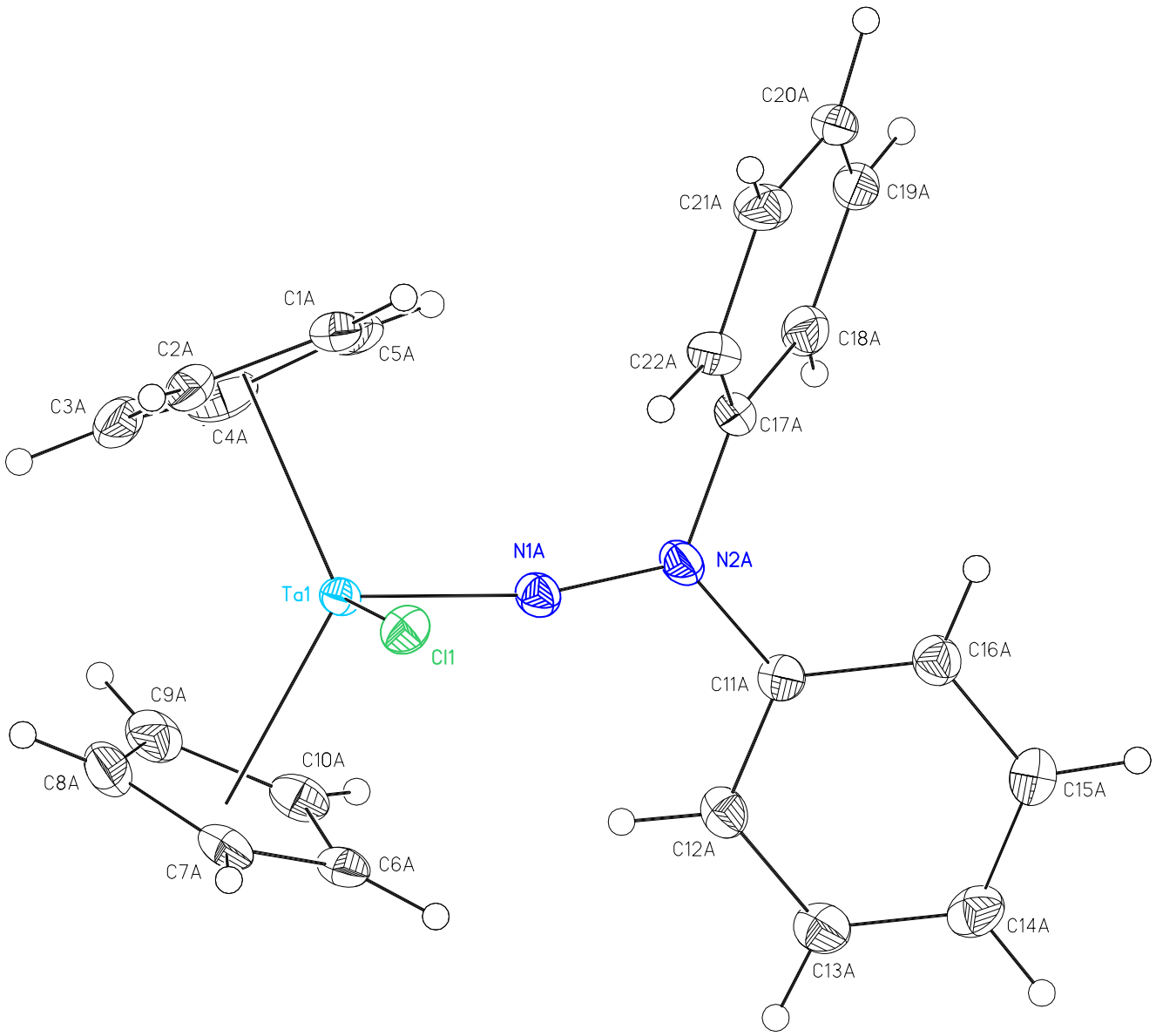
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	22998 / 0 / 629
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.495
Final R indices [$I>2\sigma(I)$, 18835 reflections]	R1 = 0.0271, *w*R2 = 0.0400
R indices (all data)	R1 = 0.0397, *w*R2 = 0.0410
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.006
Average shift/error	0.000
Largest diff. peak and hole	3.358 and -1.450 e.Å^{-3}

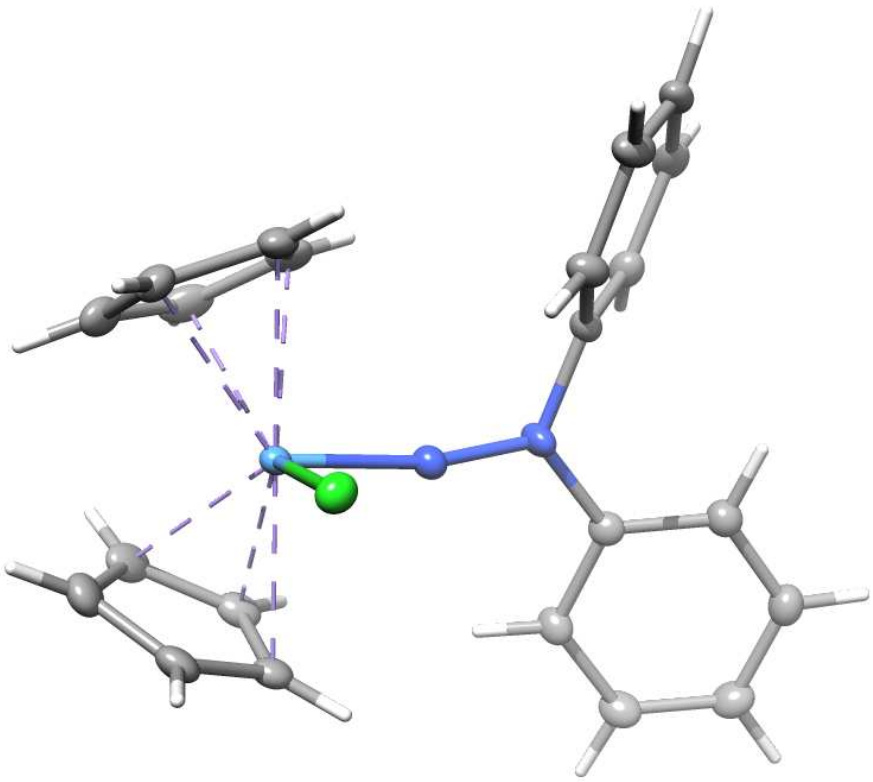
Special Refinement Details

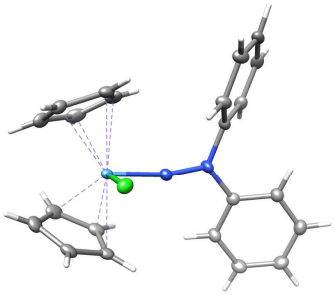
Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

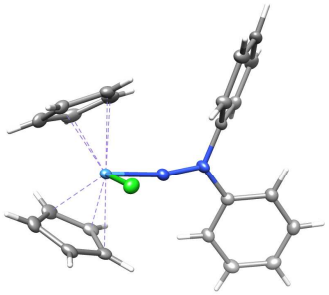
Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

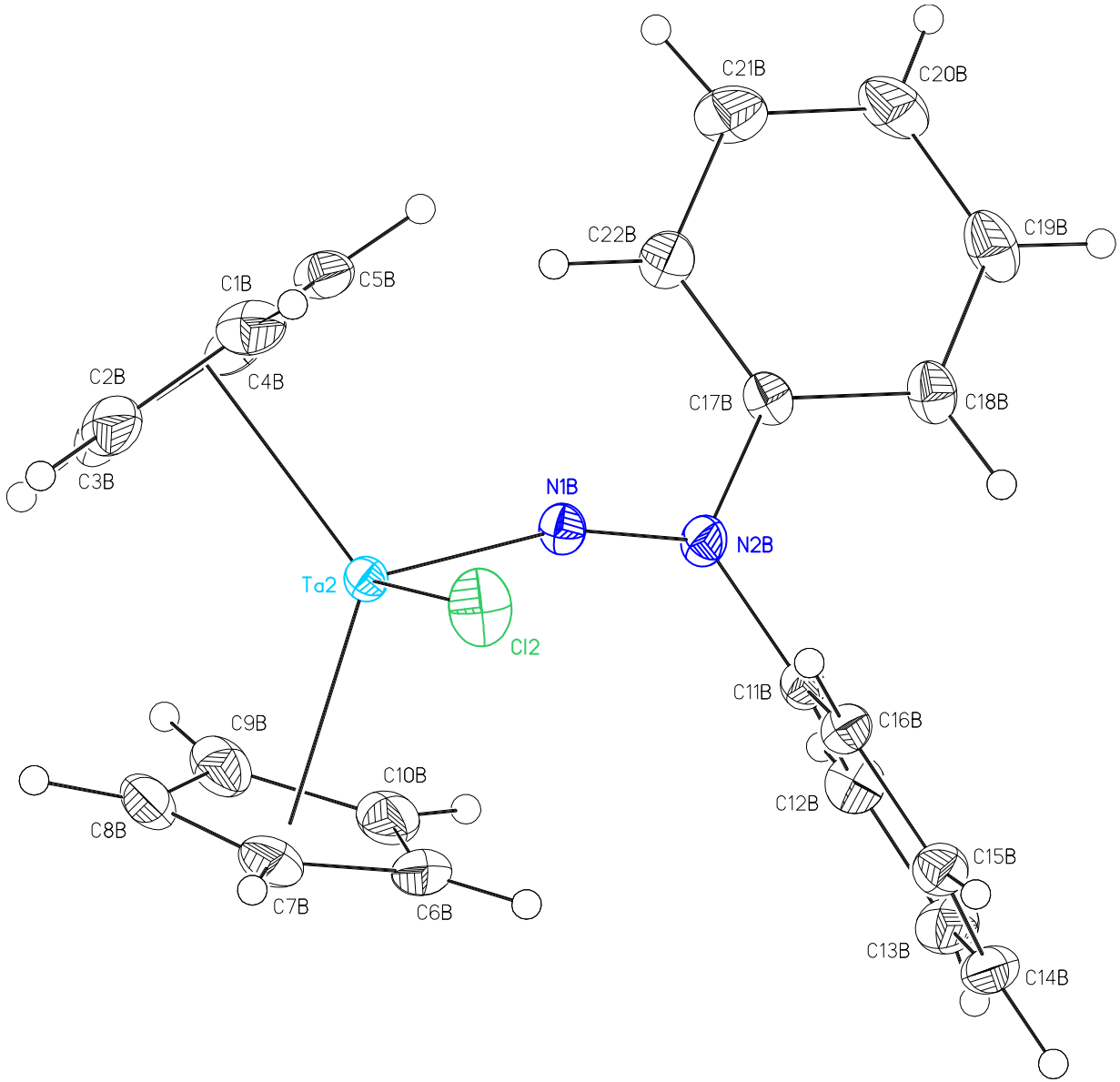
All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

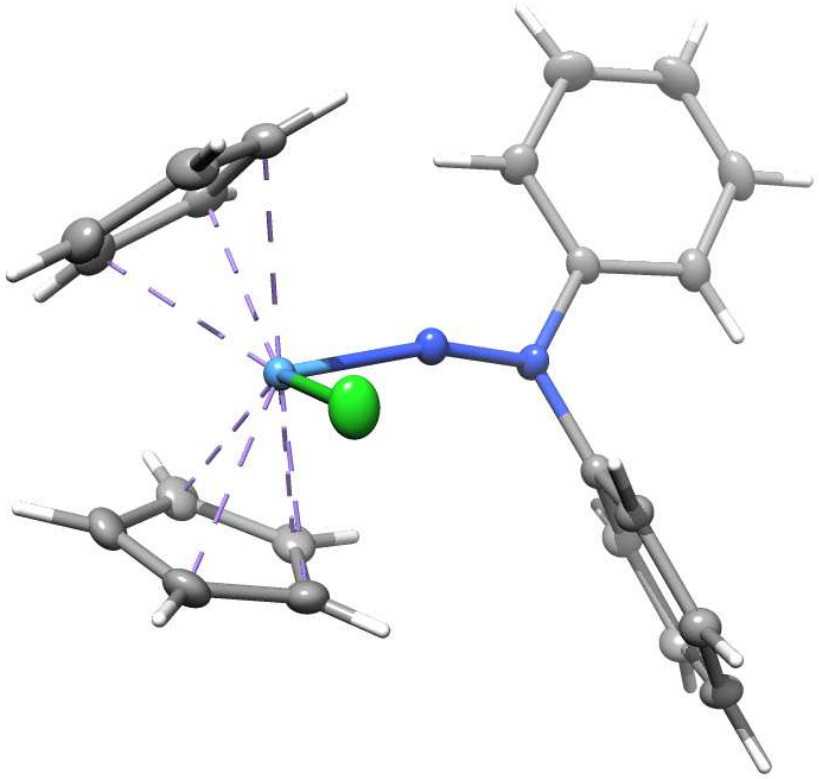

C20A
C21A
C19A
C1A
C5A
C2A
C18A
C22A
C3A
C4A
C17A
N1A
N2A
Ta1
Cl1
C16A
C11A
C9A
C10A
C15A
C8A
C12A
C7A
C6A
C14A
C13A

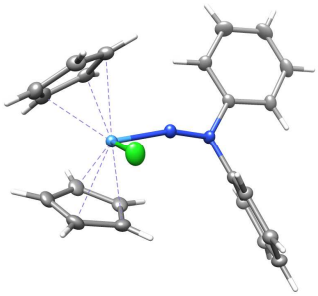


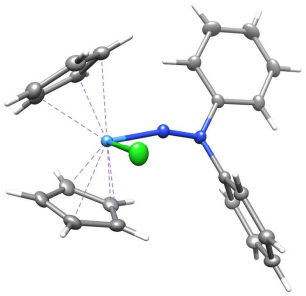


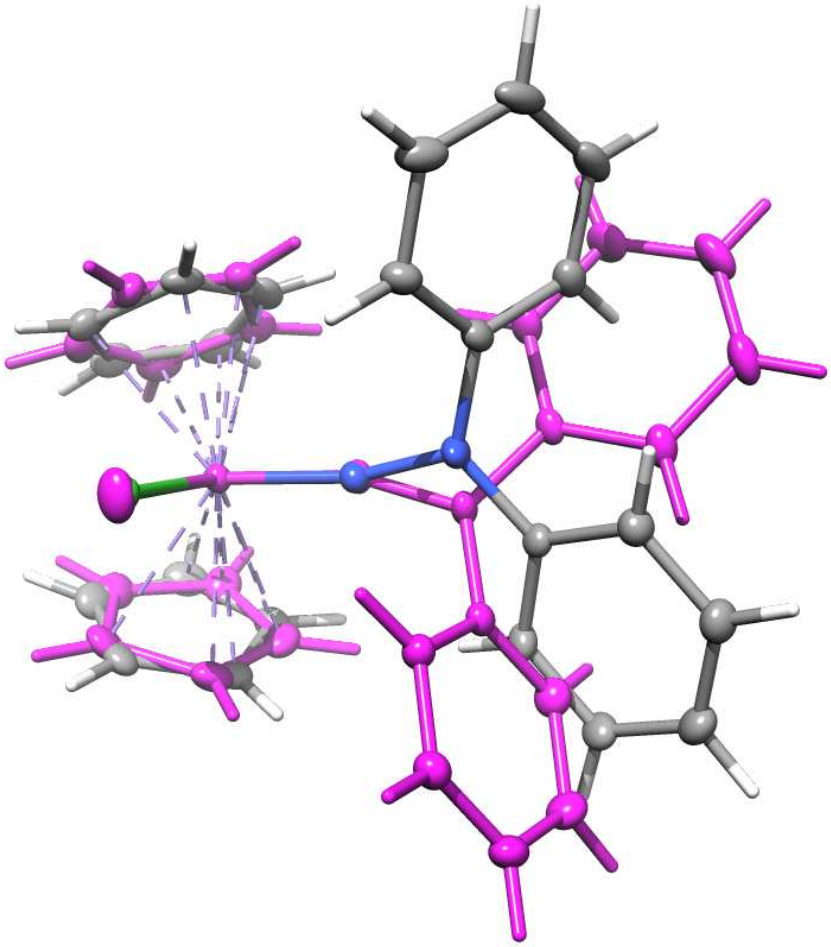



C21B
C20B
C22B
C19B
C1B
C5B
C4B
C2B
C17B
C18B
C3B
N1B
N2B
Ta2
Cl2
C11B
C16B
C9B
C10B
C12B
C8B
C15B
C7B
C6B
C13B
C14B

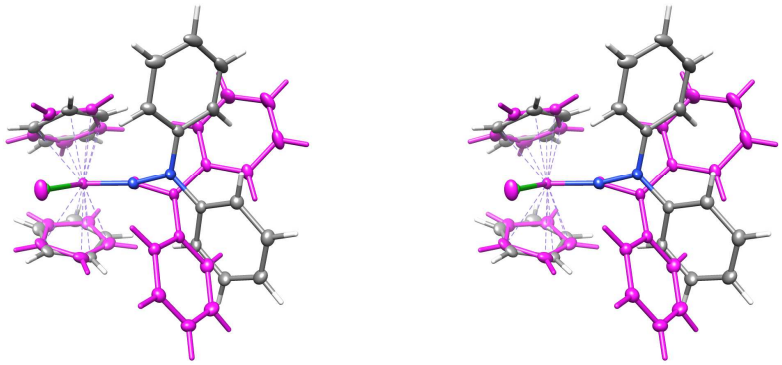


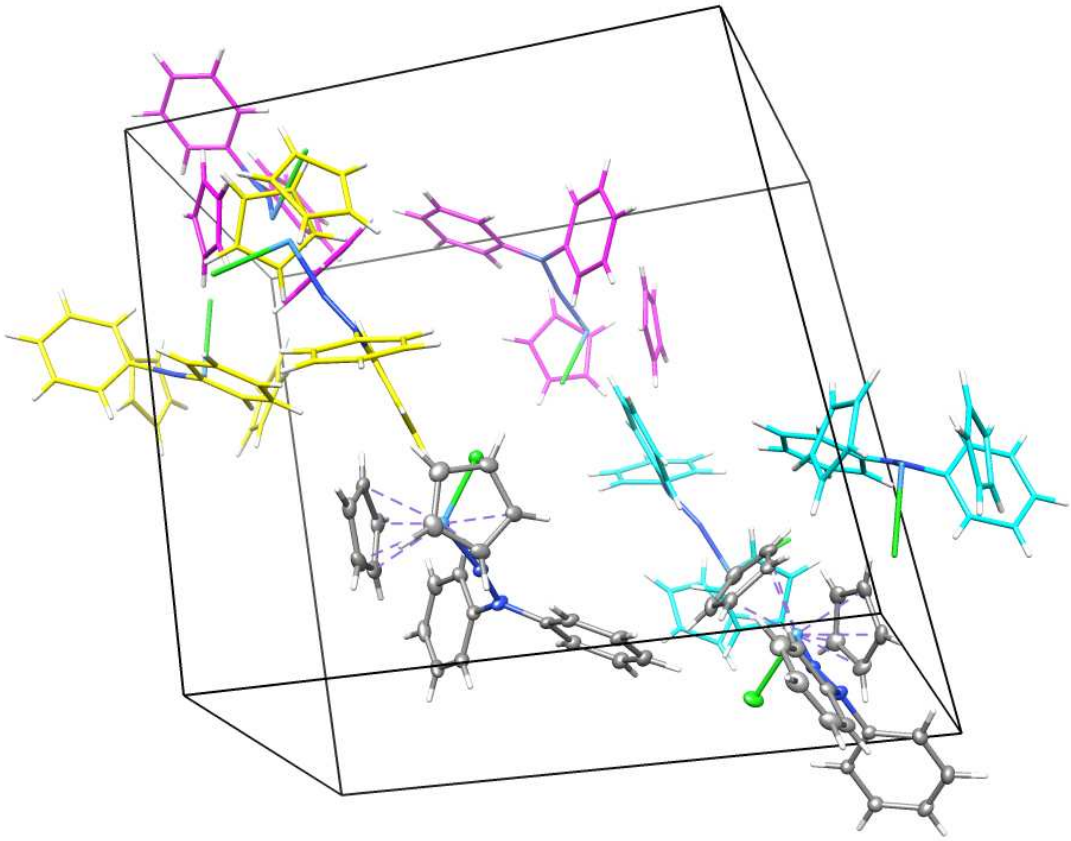


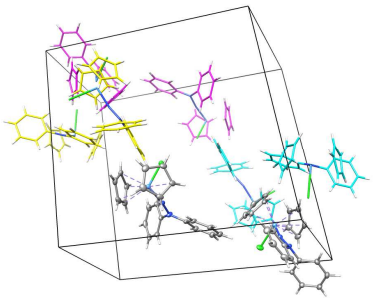




Overlap is based on Cl-Ta-N1 positions







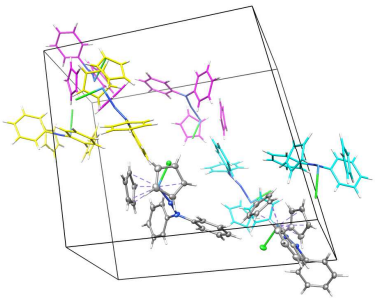


Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT49 (CCDC 767430). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	8079(1)	10849(1)	5543(1)	14(1)
Cl(1)	6903(1)	9947(1)	5046(1)	19(1)
N(1A)	8502(1)	9324(1)	5378(1)	17(1)
N(2A)	8774(1)	8122(1)	5387(1)	20(1)
C(1A)	7751(1)	10101(2)	6648(1)	24(1)
C(2A)	7448(1)	11368(2)	6529(1)	20(1)
C(3A)	8001(1)	12266(2)	6595(1)	24(1)
C(4A)	8651(1)	11566(2)	6718(1)	29(1)
C(5A)	8490(1)	10235(2)	6781(1)	30(1)
C(6A)	8253(1)	11566(2)	4381(1)	19(1)
C(7A)	7658(1)	12293(2)	4495(1)	22(1)
C(8A)	7884(1)	13180(2)	5049(1)	26(1)
C(9A)	8612(1)	12978(2)	5296(1)	26(1)
C(10A)	8849(1)	11986(2)	4880(1)	22(1)
C(11A)	9070(1)	7675(2)	4810(1)	17(1)
C(12A)	9270(1)	8573(2)	4337(1)	19(1)
C(13A)	9530(1)	8130(2)	3751(1)	23(1)
C(14A)	9603(1)	6811(2)	3634(1)	24(1)
C(15A)	9414(1)	5917(2)	4110(1)	23(1)
C(16A)	9145(1)	6342(2)	4694(1)	20(1)
C(17A)	8685(1)	7262(2)	5952(1)	17(1)
C(18A)	9280(1)	6679(2)	6359(1)	22(1)
C(19A)	9195(1)	5853(2)	6911(1)	27(1)
C(20A)	8526(1)	5631(2)	7062(1)	26(1)
C(21A)	7933(1)	6230(2)	6662(1)	25(1)
C(22A)	8011(1)	7040(2)	6098(1)	20(1)
Ta(2)	8616(1)	2394(1)	1849(1)	13(1)
Cl(2)	9343(1)	1217(1)	2833(1)	28(1)
N(1B)	9344(1)	3350(1)	1632(1)	15(1)
N(2B)	9866(1)	3786(1)	1309(1)	17(1)
C(1B)	8205(1)	3352(2)	2913(1)	25(1)
C(2B)	7610(1)	2686(2)	2535(1)	28(1)
C(3B)	7415(1)	3297(2)	1878(1)	28(1)
C(4B)	7900(1)	4332(2)	1837(1)	23(1)
C(5B)	8372(1)	4382(2)	2499(1)	21(1)
C(6B)	8898(1)	572(2)	1154(1)	27(1)
C(7B)	8343(1)	97(2)	1492(1)	27(1)
C(8B)	7726(1)	764(2)	1224(1)	25(1)
C(9B)	7887(1)	1713(2)	738(1)	26(1)
C(10B)	8605(1)	1544(2)	675(1)	26(1)
C(11B)	10336(1)	2826(2)	1112(1)	16(1)
C(12B)	10462(1)	2763(2)	421(1)	22(1)
C(13B)	10908(1)	1800(2)	242(1)	24(1)
C(14B)	11235(1)	915(2)	740(1)	22(1)
C(15B)	11119(1)	998(2)	1433(1)	20(1)
C(16B)	10668(1)	1941(2)	1618(1)	17(1)

C(17B)	10038(1)	5121(2)	1348(1)	16(1)
C(18B)	10675(1)	5585(2)	1179(1)	20(1)
C(19B)	10834(1)	6909(2)	1252(1)	26(1)
C(20B)	10380(1)	7768(2)	1493(1)	29(1)
C(21B)	9745(1)	7315(2)	1647(1)	28(1)
C(22B)	9566(1)	6001(2)	1566(1)	21(1)

Table 3. Selected bond lengths [Å] and angles [°] for IAT49 (CCDC 767430).

Ta(1)-N(1A)	1.8149(13)	N(1A)-Ta(1)-Cl(1)	90.74(4)
Ta(1)-Cl(1)	2.4544(4)		
Ta(2)-N(1B)	1.8130(13)	N(1B)-Ta(2)-Cl(2)	95.42(4)
Ta(2)-Cl(2)	2.4493(4)		

Table 4. Bond lengths [Å] and angles [°] for IAT49 (CCDC 767430).

Ta(1)-N(1A)	1.8149(13)	C(19A)-H(19A)	0.93(2)
Ta(1)-C(10A)	2.4200(16)	C(20A)-C(21A)	1.389(3)
Ta(1)-C(6A)	2.4343(13)	C(20A)-H(20A)	0.99(2)
Ta(1)-C(4A)	2.4347(16)	C(21A)-C(22A)	1.395(2)
Ta(1)-C(5A)	2.4472(15)	C(21A)-H(21A)	0.91(3)
Ta(1)-C(1A)	2.4485(15)	C(22A)-H(22A)	0.95(2)
Ta(1)-Cl(1)	2.4544(4)	Ta(2)-N(1B)	1.8130(13)
Ta(1)-C(2A)	2.4882(15)	Ta(2)-C(4B)	2.4104(17)
Ta(1)-C(9A)	2.4922(17)	Ta(2)-C(6B)	2.4146(17)
Ta(1)-C(7A)	2.5104(15)	Ta(2)-C(10B)	2.4159(15)
Ta(1)-C(3A)	2.5185(15)	Ta(2)-C(9B)	2.4267(16)
Ta(1)-C(8A)	2.5733(17)	Ta(2)-Cl(2)	2.4493(4)
N(1A)-N(2A)	1.3357(18)	Ta(2)-C(5B)	2.4801(16)
N(2A)-C(11A)	1.4138(19)	Ta(2)-C(7B)	2.4803(17)
N(2A)-C(17A)	1.4348(19)	Ta(2)-C(3B)	2.4867(19)
C(1A)-C(5A)	1.396(3)	Ta(2)-C(8B)	2.5243(17)
C(1A)-C(2A)	1.423(3)	Ta(2)-C(1B)	2.5247(15)
C(1A)-H(1A)	0.89(2)	Ta(2)-C(2B)	2.5468(18)
C(2A)-C(3A)	1.390(3)	N(1B)-N(2B)	1.3458(18)
C(2A)-H(2A)	0.84(2)	N(2B)-C(17B)	1.407(2)
C(3A)-C(4A)	1.417(3)	N(2B)-C(11B)	1.431(2)
C(3A)-H(3A)	0.95(2)	C(1B)-C(5B)	1.396(2)
C(4A)-C(5A)	1.408(3)	C(1B)-C(2B)	1.407(3)
C(4A)-H(4A)	0.95(3)	C(1B)-H(1B)	0.98(2)
C(5A)-H(5A)	0.86(3)	C(2B)-C(3B)	1.399(3)
C(6A)-C(7A)	1.412(2)	C(2B)-H(2B)	0.90(3)
C(6A)-C(10A)	1.414(2)	C(3B)-C(4B)	1.421(3)
C(6A)-H(6A)	0.95(2)	C(3B)-H(3B)	0.92(2)
C(7A)-C(8A)	1.406(3)	C(4B)-C(5B)	1.417(2)
C(7A)-H(7A)	0.93(2)	C(4B)-H(4B)	0.89(2)
C(8A)-C(9A)	1.401(3)	C(5B)-H(5B)	0.94(2)
C(8A)-H(8A)	0.91(2)	C(6B)-C(10B)	1.402(3)
C(9A)-C(10A)	1.420(3)	C(6B)-C(7B)	1.428(3)
C(9A)-H(9A)	1.03(2)	C(6B)-H(6B)	0.94(2)
C(10A)-H(10A)	0.94(2)	C(7B)-C(8B)	1.379(3)
C(11A)-C(16A)	1.396(2)	C(7B)-H(7B)	0.92(2)
C(11A)-C(12A)	1.397(2)	C(8B)-C(9B)	1.423(3)
C(12A)-C(13A)	1.390(2)	C(8B)-H(8B)	0.97(2)
C(12A)-H(12A)	0.92(2)	C(9B)-C(10B)	1.410(3)
C(13A)-C(14A)	1.382(3)	C(9B)-H(9B)	0.96(2)
C(13A)-H(13A)	0.95(2)	C(10B)-H(10B)	0.92(2)
C(14A)-C(15A)	1.389(2)	C(11B)-C(12B)	1.394(2)
C(14A)-H(14A)	0.96(2)	C(11B)-C(16B)	1.396(2)
C(15A)-C(16A)	1.390(2)	C(12B)-C(13B)	1.390(3)
C(15A)-H(15A)	0.94(2)	C(12B)-H(12B)	0.95(2)
C(16A)-H(16A)	0.95(2)	C(13B)-C(14B)	1.381(2)
C(17A)-C(22A)	1.389(2)	C(13B)-H(13B)	0.996(19)
C(17A)-C(18A)	1.390(2)	C(14B)-C(15B)	1.395(2)
C(18A)-C(19A)	1.390(2)	C(14B)-H(14B)	0.93(2)
C(18A)-H(18A)	0.95(2)	C(15B)-C(16B)	1.385(2)
C(19A)-C(20A)	1.384(3)	C(15B)-H(15B)	0.97(2)

C(16B)-H(16B)	0.976(17)	C(1A)-Ta(1)-C(7A)	141.84(6)
C(17B)-C(22B)	1.394(2)	Cl(1)-Ta(1)-C(7A)	77.02(5)
C(17B)-C(18B)	1.401(2)	C(2A)-Ta(1)-C(7A)	110.96(6)
C(18B)-C(19B)	1.392(2)	C(9A)-Ta(1)-C(7A)	53.96(6)
C(18B)-H(18B)	0.94(2)	N(1A)-Ta(1)-C(3A)	137.12(6)
C(19B)-C(20B)	1.375(3)	C(10A)-Ta(1)-C(3A)	106.17(6)
C(19B)-H(19B)	0.92(3)	C(6A)-Ta(1)-C(3A)	127.05(6)
C(20B)-C(21B)	1.383(3)	C(4A)-Ta(1)-C(3A)	33.18(7)
C(20B)-H(20B)	0.85(3)	C(5A)-Ta(1)-C(3A)	54.73(6)
C(21B)-C(22B)	1.392(2)	C(1A)-Ta(1)-C(3A)	54.54(6)
C(21B)-H(21B)	0.91(2)	Cl(1)-Ta(1)-C(3A)	110.11(5)
C(22B)-H(22B)	0.94(3)	C(2A)-Ta(1)-C(3A)	32.24(6)
		C(9A)-Ta(1)-C(3A)	74.66(6)
N(1A)-Ta(1)-C(10A)	89.29(6)	C(7A)-Ta(1)-C(3A)	104.30(6)
N(1A)-Ta(1)-C(6A)	87.55(5)	N(1A)-Ta(1)-C(8A)	140.69(6)
C(10A)-Ta(1)-C(6A)	33.87(6)	C(10A)-Ta(1)-C(8A)	54.45(6)
N(1A)-Ta(1)-C(4A)	106.56(7)	C(6A)-Ta(1)-C(8A)	54.25(6)
C(10A)-Ta(1)-C(4A)	97.56(6)	C(4A)-Ta(1)-C(8A)	94.12(7)
C(6A)-Ta(1)-C(4A)	130.31(6)	C(5A)-Ta(1)-C(8A)	126.61(6)
N(1A)-Ta(1)-C(5A)	82.90(6)	C(1A)-Ta(1)-C(8A)	124.63(6)
C(10A)-Ta(1)-C(5A)	121.32(7)	Cl(1)-Ta(1)-C(8A)	98.42(5)
C(6A)-Ta(1)-C(5A)	153.78(7)	C(2A)-Ta(1)-C(8A)	91.46(6)
C(4A)-Ta(1)-C(5A)	33.53(7)	C(9A)-Ta(1)-C(8A)	32.06(7)
N(1A)-Ta(1)-C(1A)	94.43(6)	C(7A)-Ta(1)-C(8A)	32.09(6)
C(10A)-Ta(1)-C(1A)	152.59(6)	C(3A)-Ta(1)-C(8A)	74.62(6)
C(6A)-Ta(1)-C(1A)	173.08(6)	N(2A)-N(1A)-Ta(1)	167.65(10)
C(4A)-Ta(1)-C(1A)	55.37(7)	N(1A)-N(2A)-C(11A)	120.08(12)
C(5A)-Ta(1)-C(1A)	33.13(7)	N(1A)-N(2A)-C(17A)	118.43(12)
N(1A)-Ta(1)-Cl(1)	90.74(4)	C(11A)-N(2A)-C(17A)	121.13(13)
C(10A)-Ta(1)-Cl(1)	125.40(4)	C(5A)-C(1A)-C(2A)	107.95(17)
C(6A)-Ta(1)-Cl(1)	91.59(4)	C(5A)-C(1A)-Ta(1)	73.38(9)
C(4A)-Ta(1)-Cl(1)	134.14(5)	C(2A)-C(1A)-Ta(1)	74.78(8)
C(5A)-Ta(1)-Cl(1)	112.83(6)	C(5A)-C(1A)-H(1A)	125.3(15)
C(1A)-Ta(1)-Cl(1)	81.76(5)	C(2A)-C(1A)-H(1A)	126.7(15)
N(1A)-Ta(1)-C(2A)	127.81(5)	Ta(1)-C(1A)-H(1A)	119.5(12)
C(10A)-Ta(1)-C(2A)	136.73(6)	C(3A)-C(2A)-C(1A)	108.02(18)
C(6A)-Ta(1)-C(2A)	143.55(6)	C(3A)-C(2A)-Ta(1)	75.08(9)
C(4A)-Ta(1)-C(2A)	54.92(6)	C(1A)-C(2A)-Ta(1)	71.72(9)
C(5A)-Ta(1)-C(2A)	55.01(6)	C(3A)-C(2A)-H(2A)	125.1(14)
C(1A)-Ta(1)-C(2A)	33.49(6)	C(1A)-C(2A)-H(2A)	126.8(14)
Cl(1)-Ta(1)-C(2A)	80.72(4)	Ta(1)-C(2A)-H(2A)	119.5(12)
N(1A)-Ta(1)-C(9A)	120.62(6)	C(2A)-C(3A)-C(4A)	107.96(17)
C(10A)-Ta(1)-C(9A)	33.56(6)	C(2A)-C(3A)-Ta(1)	72.68(9)
C(6A)-Ta(1)-C(9A)	55.22(6)	C(4A)-C(3A)-Ta(1)	70.16(9)
C(4A)-Ta(1)-C(9A)	77.50(6)	C(2A)-C(3A)-H(3A)	123.5(14)
C(5A)-Ta(1)-C(9A)	109.98(7)	C(4A)-C(3A)-H(3A)	128.4(14)
C(1A)-Ta(1)-C(9A)	128.29(6)	Ta(1)-C(3A)-H(3A)	120.3(11)
Cl(1)-Ta(1)-C(9A)	129.28(5)	C(5A)-C(4A)-C(3A)	107.86(18)
C(2A)-Ta(1)-C(9A)	103.40(6)	C(5A)-C(4A)-Ta(1)	73.72(10)
N(1A)-Ta(1)-C(7A)	116.99(5)	C(3A)-C(4A)-Ta(1)	76.66(9)
C(10A)-Ta(1)-C(7A)	55.12(6)	C(5A)-C(4A)-H(4A)	125.5(15)
C(6A)-Ta(1)-C(7A)	33.14(6)	C(3A)-C(4A)-H(4A)	126.6(15)
C(4A)-Ta(1)-C(7A)	126.10(7)	Ta(1)-C(4A)-H(4A)	118.1(12)
C(5A)-Ta(1)-C(7A)	158.46(6)	C(1A)-C(5A)-C(4A)	108.02(18)

C(1A)-C(5A)-Ta(1)	73.49(9)	C(22A)-C(17A)-N(2A)	119.94(14)
C(4A)-C(5A)-Ta(1)	72.75(9)	C(18A)-C(17A)-N(2A)	119.45(15)
C(1A)-C(5A)-H(5A)	125.6(18)	C(17A)-C(18A)-C(19A)	119.51(18)
C(4A)-C(5A)-H(5A)	126.3(18)	C(17A)-C(18A)-H(18A)	118.9(13)
Ta(1)-C(5A)-H(5A)	118.2(14)	C(19A)-C(18A)-H(18A)	121.6(13)
C(7A)-C(6A)-C(10A)	107.76(15)	C(20A)-C(19A)-C(18A)	120.28(17)
C(7A)-C(6A)-Ta(1)	76.39(8)	C(20A)-C(19A)-H(19A)	120.8(13)
C(10A)-C(6A)-Ta(1)	72.51(8)	C(18A)-C(19A)-H(19A)	118.9(14)
C(7A)-C(6A)-H(6A)	124.6(13)	C(19A)-C(20A)-C(21A)	120.14(15)
C(10A)-C(6A)-H(6A)	127.6(13)	C(19A)-C(20A)-H(20A)	120.7(15)
Ta(1)-C(6A)-H(6A)	115.8(12)	C(21A)-C(20A)-H(20A)	119.1(15)
C(8A)-C(7A)-C(6A)	108.44(17)	C(20A)-C(21A)-C(22A)	119.99(18)
C(8A)-C(7A)-Ta(1)	76.42(9)	C(20A)-C(21A)-H(21A)	121.7(14)
C(6A)-C(7A)-Ta(1)	70.47(8)	C(22A)-C(21A)-H(21A)	118.3(14)
C(8A)-C(7A)-H(7A)	127.1(13)	C(17A)-C(22A)-C(21A)	119.47(16)
C(6A)-C(7A)-H(7A)	124.5(13)	C(17A)-C(22A)-H(22A)	119.6(11)
Ta(1)-C(7A)-H(7A)	118.4(13)	C(21A)-C(22A)-H(22A)	120.8(11)
C(9A)-C(8A)-C(7A)	107.90(17)	N(1B)-Ta(2)-C(4B)	90.66(6)
C(9A)-C(8A)-Ta(1)	70.78(10)	N(1B)-Ta(2)-C(6B)	91.75(6)
C(7A)-C(8A)-Ta(1)	71.49(9)	C(4B)-Ta(2)-C(6B)	144.83(6)
C(9A)-C(8A)-H(8A)	125.7(13)	N(1B)-Ta(2)-C(10B)	81.59(6)
C(7A)-C(8A)-H(8A)	125.9(14)	C(4B)-Ta(2)-C(10B)	112.48(6)
Ta(1)-C(8A)-H(8A)	117.1(13)	C(6B)-Ta(2)-C(10B)	33.73(7)
C(8A)-C(9A)-C(10A)	108.44(16)	N(1B)-Ta(2)-C(9B)	107.00(6)
C(8A)-C(9A)-Ta(1)	77.16(11)	C(4B)-Ta(2)-C(9B)	89.81(7)
C(10A)-C(9A)-Ta(1)	70.43(9)	C(6B)-Ta(2)-C(9B)	56.05(7)
C(8A)-C(9A)-H(9A)	129.7(14)	C(10B)-Ta(2)-C(9B)	33.86(7)
C(10A)-C(9A)-H(9A)	121.8(14)	N(1B)-Ta(2)-Cl(2)	95.42(4)
Ta(1)-C(9A)-H(9A)	116.4(13)	C(4B)-Ta(2)-Cl(2)	130.75(4)
C(6A)-C(10A)-C(9A)	107.42(17)	C(6B)-Ta(2)-Cl(2)	83.90(5)
C(6A)-C(10A)-Ta(1)	73.62(9)	C(10B)-Ta(2)-Cl(2)	116.76(5)
C(9A)-C(10A)-Ta(1)	76.01(10)	C(9B)-Ta(2)-Cl(2)	133.65(5)
C(6A)-C(10A)-H(10A)	126.4(12)	N(1B)-Ta(2)-C(5B)	84.06(6)
C(9A)-C(10A)-H(10A)	126.2(12)	C(4B)-Ta(2)-C(5B)	33.65(6)
Ta(1)-C(10A)-H(10A)	115.1(12)	C(6B)-Ta(2)-C(5B)	175.34(6)
C(16A)-C(11A)-C(12A)	119.54(13)	C(10B)-Ta(2)-C(5B)	142.90(6)
C(16A)-C(11A)-N(2A)	120.72(13)	C(9B)-Ta(2)-C(5B)	123.30(7)
C(12A)-C(11A)-N(2A)	119.71(14)	Cl(2)-Ta(2)-C(5B)	98.49(4)
C(13A)-C(12A)-C(11A)	119.64(16)	N(1B)-Ta(2)-C(7B)	125.45(6)
C(13A)-C(12A)-H(12A)	121.4(11)	C(4B)-Ta(2)-C(7B)	133.62(7)
C(11A)-C(12A)-H(12A)	118.9(11)	C(6B)-Ta(2)-C(7B)	33.89(6)
C(14A)-C(13A)-C(12A)	120.97(15)	C(10B)-Ta(2)-C(7B)	55.53(6)
C(14A)-C(13A)-H(13A)	123.5(12)	C(9B)-Ta(2)-C(7B)	55.01(7)
C(12A)-C(13A)-H(13A)	115.5(12)	Cl(2)-Ta(2)-C(7B)	78.86(5)
C(13A)-C(14A)-C(15A)	119.43(15)	C(5B)-Ta(2)-C(7B)	150.44(6)
C(13A)-C(14A)-H(14A)	120.3(14)	N(1B)-Ta(2)-C(3B)	123.76(6)
C(15A)-C(14A)-H(14A)	120.3(14)	C(4B)-Ta(2)-C(3B)	33.68(7)
C(14A)-C(15A)-C(16A)	120.45(16)	C(6B)-Ta(2)-C(3B)	127.08(7)
C(14A)-C(15A)-H(15A)	121.3(12)	C(10B)-Ta(2)-C(3B)	107.91(7)
C(16A)-C(15A)-H(15A)	118.2(12)	C(9B)-Ta(2)-C(3B)	75.24(7)
C(15A)-C(16A)-C(11A)	119.97(15)	Cl(2)-Ta(2)-C(3B)	124.05(4)
C(15A)-C(16A)-H(16A)	120.2(13)	C(5B)-Ta(2)-C(3B)	54.65(6)
C(11A)-C(16A)-H(16A)	119.9(13)	C(7B)-Ta(2)-C(3B)	102.25(7)
C(22A)-C(17A)-C(18A)	120.60(14)	N(1B)-Ta(2)-C(8B)	136.61(5)

C(4B)-Ta(2)-C(8B)	102.09(7)	C(5B)-C(4B)-H(4B)	125.1(15)
C(6B)-Ta(2)-C(8B)	54.93(7)	C(3B)-C(4B)-H(4B)	128.0(15)
C(10B)-Ta(2)-C(8B)	55.15(6)	Ta(2)-C(4B)-H(4B)	116.2(15)
C(9B)-Ta(2)-C(8B)	33.33(6)	C(1B)-C(5B)-C(4B)	108.06(17)
Cl(2)-Ta(2)-C(8B)	106.14(4)	C(1B)-C(5B)-Ta(2)	75.58(10)
C(5B)-Ta(2)-C(8B)	127.60(6)	C(4B)-C(5B)-Ta(2)	70.48(9)
C(7B)-Ta(2)-C(8B)	31.97(7)	C(1B)-C(5B)-H(5B)	125.8(12)
C(3B)-Ta(2)-C(8B)	73.33(7)	C(4B)-C(5B)-H(5B)	126.1(12)
N(1B)-Ta(2)-C(1B)	110.18(6)	Ta(2)-C(5B)-H(5B)	116.5(14)
C(4B)-Ta(2)-C(1B)	54.88(6)	C(10B)-C(6B)-C(7B)	107.46(18)
C(6B)-Ta(2)-C(1B)	152.21(6)	C(10B)-C(6B)-Ta(2)	73.19(10)
C(10B)-Ta(2)-C(1B)	161.43(7)	C(7B)-C(6B)-Ta(2)	75.58(10)
C(9B)-Ta(2)-C(1B)	127.69(7)	C(10B)-C(6B)-H(6B)	125.7(13)
Cl(2)-Ta(2)-C(1B)	77.40(5)	C(7B)-C(6B)-H(6B)	126.8(13)
C(5B)-Ta(2)-C(1B)	32.37(5)	Ta(2)-C(6B)-H(6B)	114.4(13)
C(7B)-Ta(2)-C(1B)	120.83(6)	C(8B)-C(7B)-C(6B)	108.61(17)
C(3B)-Ta(2)-C(1B)	53.74(6)	C(8B)-C(7B)-Ta(2)	75.77(10)
C(8B)-Ta(2)-C(1B)	111.03(6)	C(6B)-C(7B)-Ta(2)	70.53(10)
N(1B)-Ta(2)-C(2B)	137.95(6)	C(8B)-C(7B)-H(7B)	123.0(16)
C(4B)-Ta(2)-C(2B)	54.90(6)	C(6B)-C(7B)-H(7B)	128.4(16)
C(6B)-Ta(2)-C(2B)	130.25(7)	Ta(2)-C(7B)-H(7B)	120.8(14)
C(10B)-Ta(2)-C(2B)	130.59(7)	C(7B)-C(8B)-C(9B)	107.99(17)
C(9B)-Ta(2)-C(2B)	97.17(7)	C(7B)-C(8B)-Ta(2)	72.26(10)
Cl(2)-Ta(2)-C(2B)	91.82(5)	C(9B)-C(8B)-Ta(2)	69.57(10)
C(5B)-Ta(2)-C(2B)	53.89(6)	C(7B)-C(8B)-H(8B)	126.5(13)
C(7B)-Ta(2)-C(2B)	96.60(6)	C(9B)-C(8B)-H(8B)	125.4(13)
C(3B)-Ta(2)-C(2B)	32.24(6)	Ta(2)-C(8B)-H(8B)	120.8(13)
C(8B)-Ta(2)-C(2B)	79.44(6)	C(10B)-C(9B)-C(8B)	107.77(18)
C(1B)-Ta(2)-C(2B)	32.22(6)	C(10B)-C(9B)-Ta(2)	72.65(9)
N(2B)-N(1B)-Ta(2)	162.28(10)	C(8B)-C(9B)-Ta(2)	77.10(9)
N(1B)-N(2B)-C(17B)	119.03(12)	C(10B)-C(9B)-H(9B)	126.8(13)
N(1B)-N(2B)-C(11B)	116.81(12)	C(8B)-C(9B)-H(9B)	125.4(13)
C(17B)-N(2B)-C(11B)	122.00(13)	Ta(2)-C(9B)-H(9B)	116.4(12)
C(5B)-C(1B)-C(2B)	108.75(16)	C(6B)-C(10B)-C(9B)	107.99(16)
C(5B)-C(1B)-Ta(2)	72.05(9)	C(6B)-C(10B)-Ta(2)	73.08(9)
C(2B)-C(1B)-Ta(2)	74.75(9)	C(9B)-C(10B)-Ta(2)	73.49(9)
C(5B)-C(1B)-H(1B)	125.6(15)	C(6B)-C(10B)-H(10B)	124.6(14)
C(2B)-C(1B)-H(1B)	125.6(15)	C(9B)-C(10B)-H(10B)	127.2(14)
Ta(2)-C(1B)-H(1B)	117.2(14)	Ta(2)-C(10B)-H(10B)	115.2(13)
C(3B)-C(2B)-C(1B)	107.64(17)	C(12B)-C(11B)-C(16B)	119.91(15)
C(3B)-C(2B)-Ta(2)	71.51(10)	C(12B)-C(11B)-N(2B)	120.87(14)
C(1B)-C(2B)-Ta(2)	73.02(10)	C(16B)-C(11B)-N(2B)	119.22(12)
C(3B)-C(2B)-H(2B)	123.9(15)	C(13B)-C(12B)-C(11B)	119.46(15)
C(1B)-C(2B)-H(2B)	128.4(15)	C(13B)-C(12B)-H(12B)	125.1(12)
Ta(2)-C(2B)-H(2B)	120.6(17)	C(11B)-C(12B)-H(12B)	115.4(12)
C(2B)-C(3B)-C(4B)	108.52(17)	C(14B)-C(13B)-C(12B)	120.96(14)
C(2B)-C(3B)-Ta(2)	76.25(11)	C(14B)-C(13B)-H(13B)	119.7(13)
C(4B)-C(3B)-Ta(2)	70.21(10)	C(12B)-C(13B)-H(13B)	119.2(13)
C(2B)-C(3B)-H(3B)	124.2(13)	C(13B)-C(14B)-C(15B)	119.39(16)
C(4B)-C(3B)-H(3B)	127.2(13)	C(13B)-C(14B)-H(14B)	120.6(11)
Ta(2)-C(3B)-H(3B)	116.7(14)	C(15B)-C(14B)-H(14B)	120.0(11)
C(5B)-C(4B)-C(3B)	106.92(15)	C(16B)-C(15B)-C(14B)	120.39(15)
C(5B)-C(4B)-Ta(2)	75.87(10)	C(16B)-C(15B)-H(15B)	119.0(12)
C(3B)-C(4B)-Ta(2)	76.11(10)	C(14B)-C(15B)-H(15B)	120.6(12)

C(15B)-C(16B)-C(11B)	119.88(13)	C(18B)-C(19B)-H(19B)	118.0(16)
C(15B)-C(16B)-H(16B)	119.0(12)	C(19B)-C(20B)-C(21B)	119.42(18)
C(11B)-C(16B)-H(16B)	121.1(12)	C(19B)-C(20B)-H(20B)	121.6(17)
C(22B)-C(17B)-C(18B)	119.32(15)	C(21B)-C(20B)-H(20B)	118.9(17)
C(22B)-C(17B)-N(2B)	119.13(14)	C(20B)-C(21B)-C(22B)	120.59(18)
C(18B)-C(17B)-N(2B)	121.56(15)	C(20B)-C(21B)-H(21B)	126.6(14)
C(19B)-C(18B)-C(17B)	119.37(17)	C(22B)-C(21B)-H(21B)	112.8(14)
C(19B)-C(18B)-H(18B)	119.7(15)	C(21B)-C(22B)-C(17B)	119.99(17)
C(17B)-C(18B)-H(18B)	120.9(15)	C(21B)-C(22B)-H(22B)	119.2(15)
C(20B)-C(19B)-C(18B)	121.23(18)	C(17B)-C(22B)-H(22B)	120.8(15)
C(20B)-C(19B)-H(19B)	120.7(15)		

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT49 (CCDC 767430). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	150(1)	136(1)	130(1)	18(1)	36(1)	7(1)
Cl(1)	174(2)	210(2)	189(1)	-19(1)	46(1)	-17(1)
N(1A)	164(7)	168(6)	181(5)	24(4)	48(4)	20(5)
N(2A)	235(8)	166(6)	215(5)	58(4)	97(5)	69(5)
C(1A)	364(11)	217(8)	150(6)	18(5)	95(6)	-5(7)
C(2A)	217(9)	230(8)	171(6)	-30(5)	74(6)	1(7)
C(3A)	328(10)	217(8)	193(6)	-63(6)	66(6)	-58(7)
C(4A)	230(10)	472(12)	171(6)	-43(7)	18(6)	-66(9)
C(5A)	373(12)	383(11)	125(6)	28(6)	25(6)	145(9)
C(6A)	202(8)	211(7)	171(6)	62(5)	54(5)	2(6)
C(7A)	213(9)	213(8)	223(6)	98(6)	33(6)	26(6)
C(8A)	330(11)	164(7)	302(8)	51(6)	103(7)	24(7)
C(9A)	334(11)	193(8)	257(7)	34(6)	44(7)	-92(7)
C(10A)	175(9)	250(8)	239(7)	84(6)	48(6)	-20(7)
C(11A)	122(7)	200(7)	186(6)	14(5)	43(5)	27(6)
C(12A)	152(8)	188(7)	251(7)	30(5)	72(6)	36(6)
C(13A)	183(9)	275(9)	256(7)	55(6)	100(6)	37(7)
C(14A)	206(9)	315(9)	220(7)	-8(6)	80(6)	42(7)
C(15A)	235(9)	207(8)	259(7)	-32(6)	55(6)	17(7)
C(16A)	202(9)	195(7)	221(6)	11(5)	53(6)	10(6)
C(17A)	210(8)	145(6)	165(5)	18(5)	40(5)	26(6)
C(18A)	237(9)	217(8)	193(6)	-9(5)	25(6)	61(7)
C(19A)	402(12)	223(8)	151(6)	3(5)	-14(6)	128(8)
C(20A)	490(13)	157(7)	148(6)	14(5)	59(6)	-12(7)
C(21A)	329(11)	235(8)	194(6)	2(6)	70(6)	-97(7)
C(22A)	211(9)	220(8)	172(6)	36(5)	25(6)	-16(6)
Ta(2)	137(1)	118(1)	152(1)	13(1)	38(1)	-7(1)
Cl(2)	260(2)	287(2)	282(2)	142(2)	11(2)	15(2)
N(1B)	152(7)	143(6)	170(5)	33(4)	36(4)	-2(5)
N(2B)	160(7)	135(6)	226(5)	28(4)	78(5)	-8(5)
C(1B)	359(11)	216(8)	194(6)	5(5)	129(7)	-7(7)
C(2B)	300(10)	240(9)	354(8)	-10(7)	201(8)	-31(8)
C(3B)	170(9)	340(10)	344(8)	-71(7)	57(7)	56(7)
C(4B)	250(9)	219(8)	229(6)	32(6)	82(6)	98(7)
C(5B)	267(9)	170(7)	217(6)	-17(5)	103(6)	5(6)
C(6B)	264(10)	181(8)	386(9)	-92(6)	107(7)	-6(7)
C(7B)	318(11)	140(7)	370(9)	-39(6)	83(7)	-62(7)
C(8B)	240(10)	248(9)	276(7)	-74(6)	54(6)	-97(7)
C(9B)	268(10)	304(9)	196(6)	-48(6)	15(6)	-71(8)
C(10B)	309(10)	293(9)	207(7)	-90(6)	98(7)	-79(8)
C(11B)	149(7)	139(6)	184(6)	8(5)	41(5)	-17(5)
C(12B)	242(9)	234(8)	180(6)	28(5)	37(6)	5(7)
C(13B)	286(10)	267(9)	184(6)	-22(6)	79(6)	4(7)
C(14B)	244(9)	178(7)	263(7)	-36(6)	97(6)	13(6)
C(15B)	215(9)	167(7)	216(6)	12(5)	47(6)	3(6)
C(16B)	183(8)	160(7)	169(6)	15(5)	53(5)	8(6)

C(17B)	169(8)	138(6)	160(5)	49(4)	7(5)	-11(5)
C(18B)	171(8)	193(7)	239(6)	66(5)	21(6)	-16(6)
C(19B)	224(10)	219(8)	330(8)	87(6)	6(7)	-72(7)
C(20B)	345(12)	151(8)	360(9)	38(6)	3(8)	-56(7)
C(21B)	372(12)	142(7)	326(8)	51(6)	97(8)	39(7)
C(22B)	218(9)	152(7)	257(7)	62(5)	70(6)	15(6)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for IAT49 (CCDC 767430).

	x	y	z	U_{iso}
H(1A)	7516(12)	9350(20)	6654(9)	23(5)
H(2A)	7015(12)	11550(20)	6439(9)	15(5)
H(3A)	7930(12)	13180(20)	6538(9)	26(5)
H(4A)	9115(14)	11920(20)	6774(10)	35(6)
H(5A)	8791(14)	9610(30)	6872(11)	36(6)
H(6A)	8238(12)	10900(20)	4035(9)	21(5)
H(7A)	7199(13)	12180(20)	4244(10)	25(5)
H(8A)	7597(12)	13710(20)	5251(10)	25(5)
H(9A)	8948(14)	13410(20)	5712(11)	40(6)
H(10A)	9314(13)	11660(20)	4935(9)	23(5)
H(12A)	9232(11)	9450(20)	4425(9)	19(5)
H(13A)	9644(11)	8790(20)	3443(9)	20(5)
H(14A)	9768(13)	6520(20)	3222(11)	35(6)
H(15A)	9480(12)	5010(20)	4057(10)	26(5)
H(16A)	9012(13)	5730(20)	5016(10)	30(5)
H(18A)	9739(13)	6880(20)	6261(10)	29(5)
H(19A)	9596(13)	5480(20)	7184(10)	26(5)
H(20A)	8465(14)	5080(20)	7468(11)	42(6)
H(21A)	7484(14)	6080(20)	6744(10)	31(6)
H(22A)	7615(11)	7486(18)	5836(9)	14(4)
H(1B)	8472(14)	3110(20)	3380(12)	40(6)
H(2B)	7382(15)	1990(30)	2672(12)	45(7)
H(3B)	7048(13)	3020(20)	1527(10)	28(5)
H(4B)	7905(13)	4880(20)	1482(10)	31(6)
H(5B)	8754(13)	4970(20)	2625(10)	30(6)
H(6B)	9381(13)	320(20)	1252(10)	28(5)
H(7B)	8366(14)	-550(20)	1825(11)	37(6)
H(8B)	7269(14)	650(20)	1362(10)	31(6)
H(9B)	7561(13)	2350(20)	498(10)	23(5)
H(10B)	8858(12)	2030(20)	401(10)	25(5)
H(12B)	10220(12)	3400(20)	105(10)	28(5)
H(13B)	10958(12)	1700(20)	-262(10)	28(5)
H(14B)	11538(12)	280(20)	619(9)	20(5)
H(15B)	11370(12)	420(20)	1798(9)	23(5)
H(16B)	10581(11)	1960(20)	2102(9)	19(5)
H(18B)	10994(13)	5020(20)	1018(10)	31(6)
H(19B)	11261(15)	7190(20)	1152(11)	38(6)
H(20B)	10470(14)	8580(30)	1529(11)	36(6)
H(21B)	9412(13)	7800(20)	1817(10)	26(5)
H(22B)	9118(15)	5720(20)	1645(11)	42(6)

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 5 February 2009

Crystal Structure Analysis of:

Complex 8 (IAT30)

(shown below)

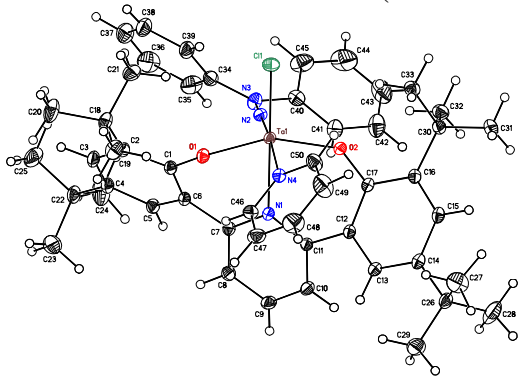
For Investigator: Ian Tonks ext. 6576

Advisor: J. E. Bercaw ext. 6577

By Michael W. Day 116 Beckman ext. 2734

e-mail: mikeday@caltech.edu

Contents



IAT30

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC). The deposition number is 719322.

Table 1. Crystal data and structure refinement for IAT30 (CCDC 719322).

Empirical formula	$C_{50}H_{58}N_4O_2ClTa$
Formula weight	963.40
Crystallization Solvent	Dichloromethane/pentane
Crystal Habit	Fragment
Crystal size	0.28 x 0.18 x 0.15 mm^3
Crystal color	Orange

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9888 reflections used in lattice determination	2.54 to 39.73°
Unit cell dimensions	a = 15.6102(8) Å b = 20.2128(10) Å β= 113.066(3)° c = 15.7963(8) Å
Volume	4585.7(4) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.395 Mg/m^3
F(000)	1968
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	1.73 to 40.11°
Completeness to θ = 40.11°	90.7 %
Index ranges	$-27 \le h \le 25$, $-36 \le k \le 35$, $-28 \le l \le 15$
Data collection scan type	ω scans; 18 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	173366
Independent reflections	25988 [R_{int}= 0.0352]
Absorption coefficient	2.498 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7479 and 0.6219

Table 1 (cont.)

Structure solution and Refinement

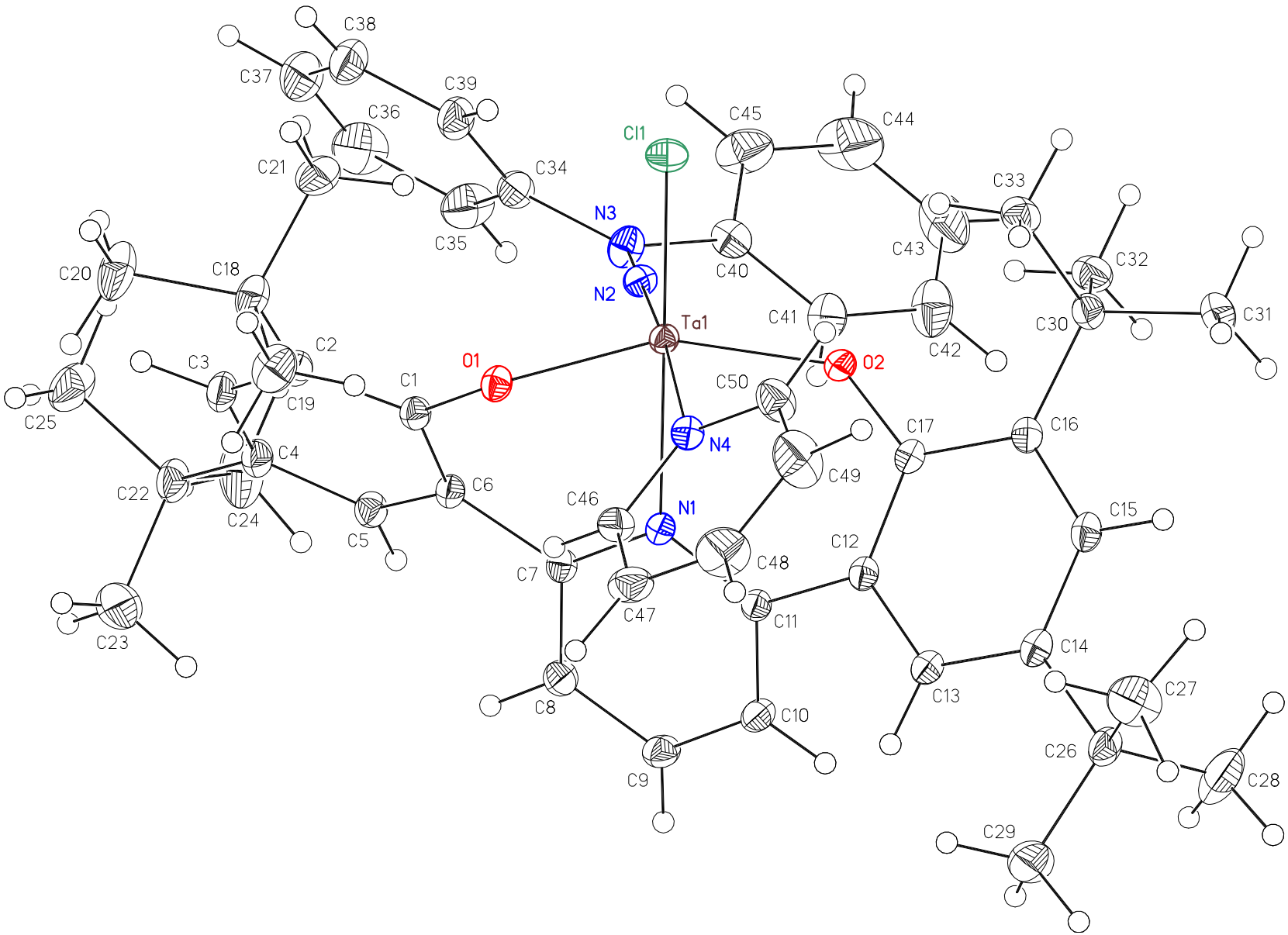
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	25988 / 0 / 755
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.718
Final R indices [$I>2\sigma(I)$, 20737 reflections]	R1 = 0.0250, *w*R2 = 0.0380
R indices (all data)	R1 = 0.0414, *w*R2 = 0.0390
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	2.328 and -1.386 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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N2
Ta1
C41
C30
C31
C2
O1
C3
C1
C19
C50
O2
C42
C25
C4
N4
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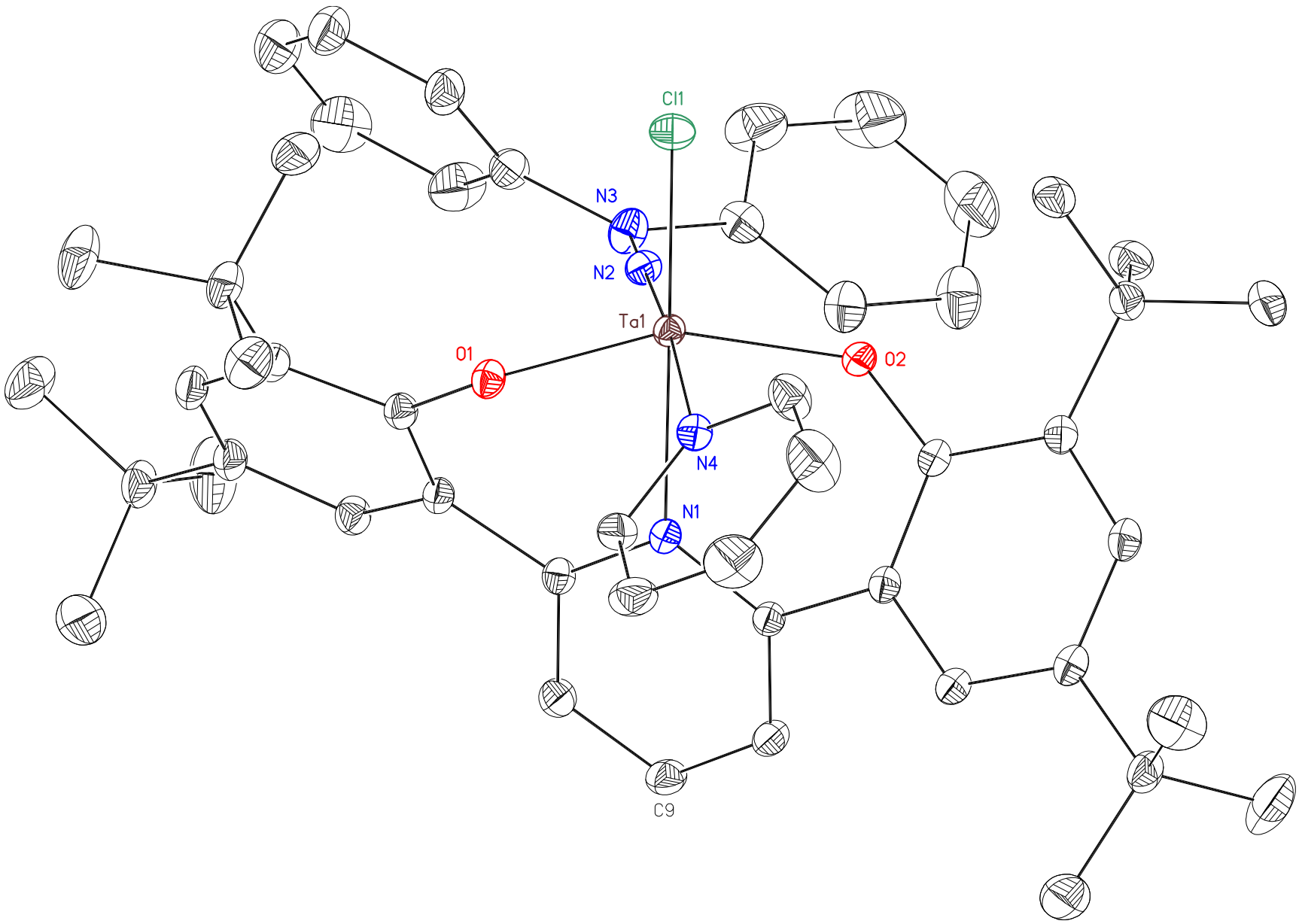
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Ta1
O1
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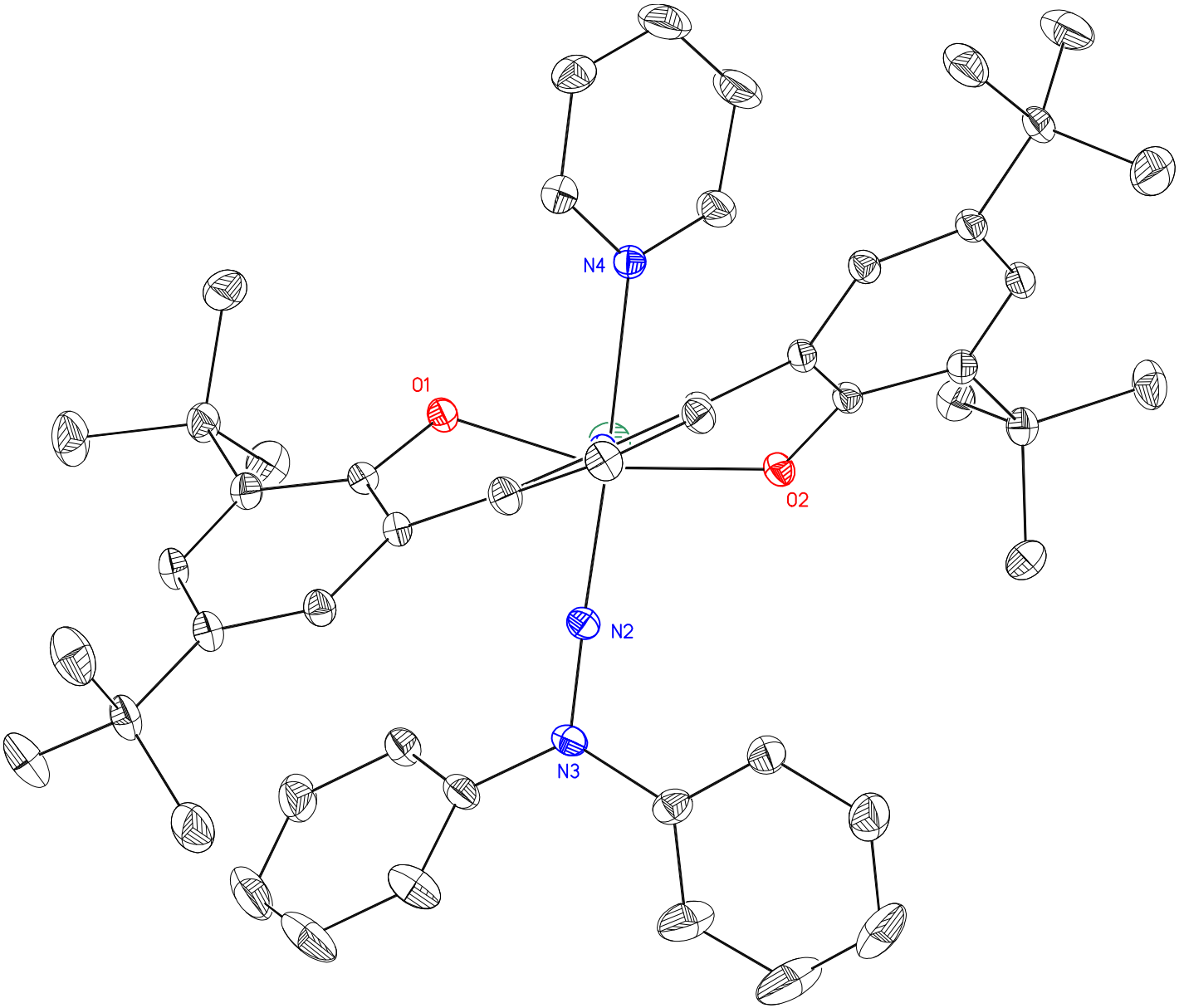
N4
N1
C9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O1
O2
N2
N3

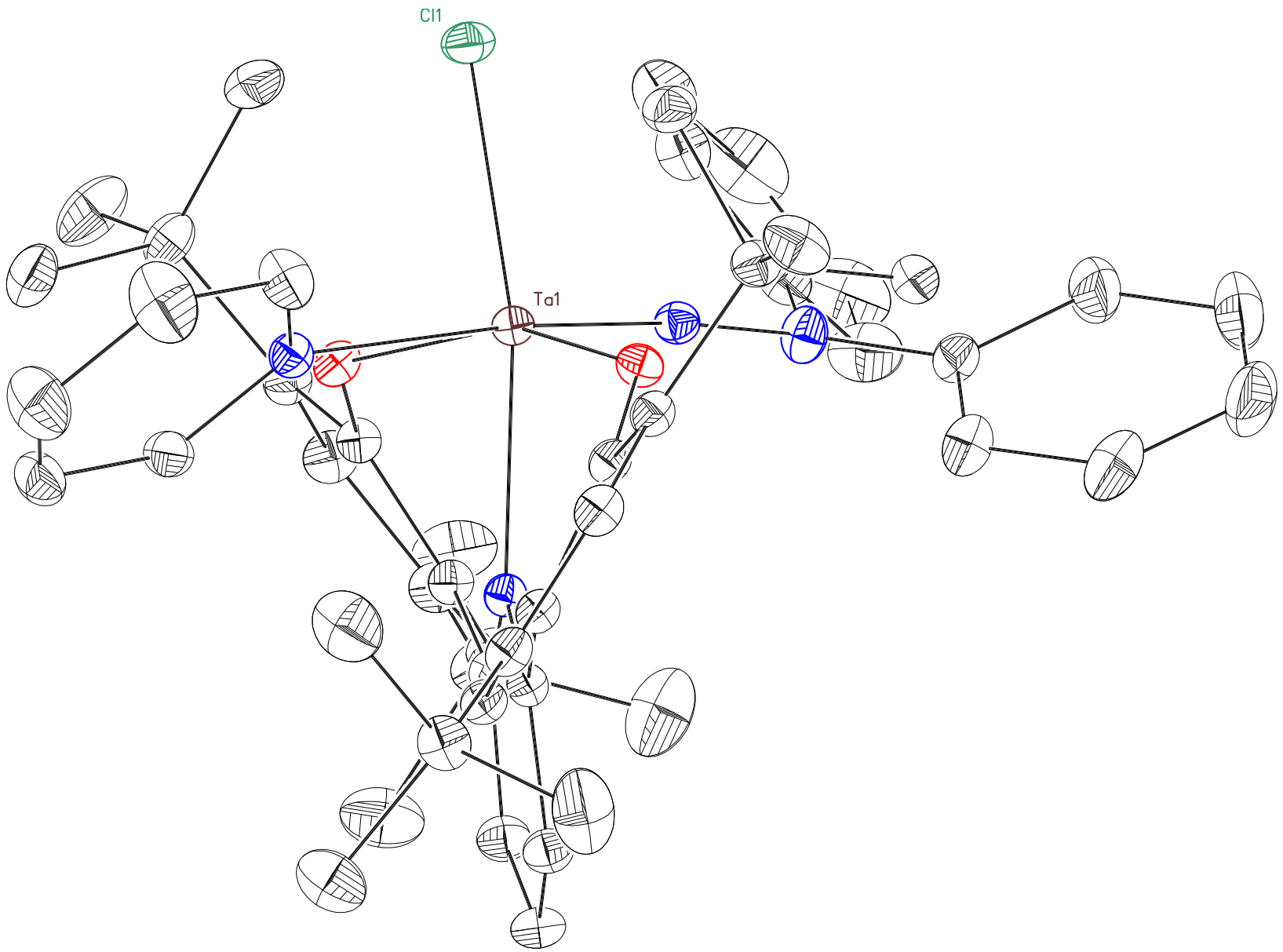
Cl1
Ta1

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT30 (CCDC 719322). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	496(1)	2071(1)	1884(1)	12(1)
Cl(1)	-107(1)	2901(1)	2589(1)	19(1)
O(1)	1533(1)	2607(1)	1832(1)	14(1)
O(2)	-621(1)	1495(1)	1376(1)	14(1)
N(1)	946(1)	1438(1)	963(1)	13(1)
N(2)	1140(1)	1574(1)	2869(1)	14(1)
N(3)	1623(1)	1153(1)	3557(1)	18(1)
N(4)	-256(1)	2683(1)	520(1)	14(1)
C(1)	2418(1)	2388(1)	2154(1)	14(1)
C(2)	3160(1)	2812(1)	2680(1)	16(1)
C(3)	4041(1)	2526(1)	3077(1)	19(1)
C(4)	4229(1)	1862(1)	2968(1)	18(1)
C(5)	3497(1)	1481(1)	2380(1)	16(1)
C(6)	2593(1)	1738(1)	1945(1)	14(1)
C(7)	1881(1)	1345(1)	1200(1)	13(1)
C(8)	2196(1)	897(1)	714(1)	17(1)
C(9)	1564(1)	524(1)	8(1)	17(1)
C(10)	629(1)	635(1)	-244(1)	16(1)
C(11)	318(1)	1106(1)	217(1)	13(1)
C(12)	-700(1)	1203(1)	-104(1)	13(1)
C(13)	-1248(1)	1122(1)	-1052(1)	15(1)
C(14)	-2205(1)	1116(1)	-1387(1)	16(1)
C(15)	-2623(1)	1155(1)	-744(1)	16(1)
C(16)	-2123(1)	1251(1)	198(1)	15(1)
C(17)	-1149(1)	1322(1)	499(1)	13(1)
C(18)	2991(1)	3548(1)	2804(1)	20(1)
C(19)	2490(1)	3880(1)	1861(1)	26(1)
C(20)	3908(1)	3923(1)	3294(1)	32(1)
C(21)	2401(1)	3631(1)	3381(1)	24(1)
C(22)	5209(1)	1564(1)	3428(1)	21(1)
C(23)	5653(1)	1533(1)	2723(1)	34(1)
C(24)	5172(1)	860(1)	3784(1)	38(1)
C(25)	5825(1)	1978(1)	4260(1)	32(1)
C(26)	-2826(1)	1064(1)	-2421(1)	18(1)
C(27)	-3527(1)	1638(1)	-2690(1)	33(1)
C(28)	-3346(1)	408(1)	-2615(1)	39(1)
C(29)	-2263(1)	1116(1)	-3027(1)	28(1)
C(30)	-2617(1)	1264(1)	874(1)	17(1)
C(31)	-3661(1)	1122(1)	391(1)	26(1)
C(32)	-2198(1)	726(1)	1609(1)	20(1)
C(33)	-2515(1)	1944(1)	1343(1)	20(1)
C(34)	2430(1)	1405(1)	4284(1)	19(1)
C(35)	3186(1)	992(1)	4728(1)	30(1)
C(36)	3969(1)	1243(1)	5445(1)	38(1)
C(37)	4001(1)	1896(1)	5712(1)	36(1)
C(38)	3256(1)	2307(1)	5261(1)	29(1)
C(39)	2467(1)	2063(1)	4545(1)	22(1)

C(40)	1158(1)	572(1)	3642(1)	19(1)
C(41)	502(1)	278(1)	2852(1)	22(1)
C(42)	22(1)	-278(1)	2921(1)	30(1)
C(43)	178(1)	-552(1)	3773(1)	39(1)
C(44)	815(1)	-255(1)	4551(1)	45(1)
C(45)	1305(1)	297(1)	4498(1)	33(1)
C(46)	195(1)	2859(1)	-20(1)	18(1)
C(47)	-238(1)	3195(1)	-843(1)	23(1)
C(48)	-1164(1)	3340(1)	-1131(1)	32(1)
C(49)	-1638(1)	3162(1)	-591(1)	34(1)
C(50)	-1156(1)	2842(1)	238(1)	22(1)

Table 3. Selected bond lengths [Å] and angles [°] for IAT30 (CCDC 719322).

Ta(1)-N(2)	1.7925(8)	N(2)-Ta(1)-O(1)	98.81(4)
Ta(1)-O(1)	1.9763(8)	N(2)-Ta(1)-O(2)	97.34(4)
Ta(1)-O(2)	1.9856(8)	O(1)-Ta(1)-O(2)	155.33(3)
Ta(1)-N(1)	2.2457(9)	N(2)-Ta(1)-N(1)	91.85(4)
Ta(1)-N(4)	2.3598(8)	O(1)-Ta(1)-N(1)	79.40(3)
Ta(1)-Cl(1)	2.4010(3)	O(2)-Ta(1)-N(1)	81.56(3)
		N(2)-Ta(1)-N(4)	174.40(4)
		O(1)-Ta(1)-N(4)	78.29(3)
		O(2)-Ta(1)-N(4)	83.93(3)
		N(1)-Ta(1)-N(4)	82.93(3)
		N(2)-Ta(1)-Cl(1)	100.20(3)
		O(1)-Ta(1)-Cl(1)	96.48(2)
		O(2)-Ta(1)-Cl(1)	98.88(2)
		N(1)-Ta(1)-Cl(1)	167.76(2)
		N(4)-Ta(1)-Cl(1)	84.96(2)

Table 4. Bond lengths [Å] and angles [°] for IAT30 (CCDC 719322).

Ta(1)-N(2)	1.7925(8)	C(20)-H(20B)	0.967(17)
Ta(1)-O(1)	1.9763(8)	C(20)-H(20C)	0.964(15)
Ta(1)-O(2)	1.9856(8)	C(21)-H(21A)	0.953(15)
Ta(1)-N(1)	2.2457(9)	C(21)-H(21B)	0.951(16)
Ta(1)-N(4)	2.3598(8)	C(21)-H(21C)	0.951(13)
Ta(1)-Cl(1)	2.4010(3)	C(22)-C(23)	1.5260(18)
O(1)-C(1)	1.3454(13)	C(22)-C(25)	1.5366(17)
O(2)-C(17)	1.3523(11)	C(22)-C(24)	1.539(2)
N(1)-C(7)	1.3705(13)	C(23)-H(23A)	1.006(17)
N(1)-C(11)	1.3767(12)	C(23)-H(23B)	1.009(17)
N(2)-N(3)	1.3546(12)	C(23)-H(23C)	1.062(17)
N(3)-C(40)	1.4135(16)	C(24)-H(24A)	1.036(18)
N(3)-C(34)	1.4254(14)	C(24)-H(24B)	1.052(18)
N(4)-C(50)	1.3367(14)	C(24)-H(24C)	1.020(16)
N(4)-C(46)	1.3497(14)	C(25)-H(25A)	0.985(17)
C(1)-C(6)	1.4076(16)	C(25)-H(25B)	0.977(16)
C(1)-C(2)	1.4180(15)	C(25)-H(25C)	0.991(16)
C(2)-C(3)	1.3939(16)	C(26)-C(28)	1.5214(19)
C(2)-C(18)	1.5373(16)	C(26)-C(27)	1.5360(19)
C(3)-C(4)	1.4002(18)	C(26)-C(29)	1.5362(17)
C(3)-H(3)	0.958(14)	C(27)-H(27A)	1.010(13)
C(4)-C(5)	1.3888(15)	C(27)-H(27B)	0.99(2)
C(4)-C(22)	1.5355(16)	C(27)-H(27C)	1.037(17)
C(5)-C(6)	1.4039(15)	C(28)-H(28A)	1.004(15)
C(5)-H(5)	0.956(13)	C(28)-H(28B)	1.06(2)
C(6)-C(7)	1.4927(14)	C(28)-H(28C)	1.043(14)
C(7)-C(8)	1.3958(15)	C(29)-H(29A)	1.005(12)
C(8)-C(9)	1.3867(15)	C(29)-H(29B)	1.013(17)
C(8)-H(8)	0.947(13)	C(29)-H(29C)	1.086(17)
C(9)-C(10)	1.3719(16)	C(30)-C(31)	1.5312(16)
C(9)-H(9)	0.925(13)	C(30)-C(32)	1.5381(17)
C(10)-C(11)	1.3955(15)	C(30)-C(33)	1.5385(17)
C(10)-H(10)	0.916(13)	C(31)-H(31A)	0.953(16)
C(11)-C(12)	1.4801(14)	C(31)-H(31B)	0.982(16)
C(12)-C(17)	1.4067(14)	C(31)-H(31C)	0.947(14)
C(12)-C(13)	1.4130(13)	C(32)-H(32A)	0.977(13)
C(13)-C(14)	1.3752(15)	C(32)-H(32B)	0.947(13)
C(13)-H(13)	0.948(11)	C(32)-H(32C)	0.961(16)
C(14)-C(15)	1.4086(15)	C(33)-H(33A)	0.935(15)
C(14)-C(26)	1.5417(13)	C(33)-H(33B)	0.955(14)
C(15)-C(16)	1.3971(13)	C(33)-H(33C)	0.970(13)
C(15)-H(15)	0.931(12)	C(34)-C(39)	1.3878(18)
C(16)-C(17)	1.4114(14)	C(34)-C(35)	1.3908(18)
C(16)-C(30)	1.5437(14)	C(35)-C(36)	1.397(2)
C(18)-C(20)	1.5341(18)	C(35)-H(35)	0.887(14)
C(18)-C(19)	1.5394(16)	C(36)-C(37)	1.379(2)
C(18)-C(21)	1.5381(17)	C(36)-H(36)	0.938(17)
C(19)-H(19A)	0.947(15)	C(37)-C(38)	1.380(2)
C(19)-H(19B)	0.935(15)	C(37)-H(37)	0.964(17)
C(19)-H(19C)	0.915(15)	C(38)-C(39)	1.3951(16)
C(20)-H(20A)	0.938(14)	C(38)-H(38)	0.930(16)

C(39)-H(39)	0.968(14)	C(1)-C(2)-C(18)	121.21(10)
C(40)-C(45)	1.3954(15)	C(2)-C(3)-C(4)	124.01(10)
C(40)-C(41)	1.3984(16)	C(2)-C(3)-H(3)	118.7(8)
C(41)-C(42)	1.3794(19)	C(4)-C(3)-H(3)	117.3(8)
C(41)-H(41)	0.956(13)	C(5)-C(4)-C(3)	117.12(10)
C(42)-C(43)	1.385(2)	C(5)-C(4)-C(22)	120.40(11)
C(42)-H(42)	0.928(16)	C(3)-C(4)-C(22)	122.38(10)
C(43)-C(44)	1.380(2)	C(4)-C(5)-C(6)	121.92(11)
C(43)-H(43)	0.904(16)	C(4)-C(5)-H(5)	119.3(7)
C(44)-C(45)	1.374(2)	C(6)-C(5)-H(5)	118.8(7)
C(44)-H(44)	0.965(17)	C(5)-C(6)-C(1)	118.74(9)
C(45)-H(45)	0.986(14)	C(5)-C(6)-C(7)	118.97(10)
C(46)-C(47)	1.3849(15)	C(1)-C(6)-C(7)	121.90(9)
C(46)-H(46)	0.932(13)	N(1)-C(7)-C(8)	120.43(9)
C(47)-C(48)	1.3653(19)	N(1)-C(7)-C(6)	121.79(9)
C(47)-H(47)	0.981(14)	C(8)-C(7)-C(6)	117.71(10)
C(48)-C(49)	1.378(2)	C(9)-C(8)-C(7)	120.09(10)
C(48)-H(48)	0.980(16)	C(9)-C(8)-H(8)	119.8(7)
C(49)-C(50)	1.3881(16)	C(7)-C(8)-H(8)	120.1(7)
C(49)-H(49)	0.938(17)	C(10)-C(9)-C(8)	119.04(11)
C(50)-H(50)	0.972(12)	C(10)-C(9)-H(9)	121.1(8)
		C(8)-C(9)-H(9)	119.8(8)
N(2)-Ta(1)-O(1)	98.81(4)	C(9)-C(10)-C(11)	120.54(10)
N(2)-Ta(1)-O(2)	97.34(4)	C(9)-C(10)-H(10)	118.9(9)
O(1)-Ta(1)-O(2)	155.33(3)	C(11)-C(10)-H(10)	120.5(9)
N(2)-Ta(1)-N(1)	91.85(4)	N(1)-C(11)-C(10)	120.18(10)
O(1)-Ta(1)-N(1)	79.40(3)	N(1)-C(11)-C(12)	122.48(9)
O(2)-Ta(1)-N(1)	81.56(3)	C(10)-C(11)-C(12)	117.28(9)
N(2)-Ta(1)-N(4)	174.40(4)	C(17)-C(12)-C(13)	118.78(9)
O(1)-Ta(1)-N(4)	78.29(3)	C(17)-C(12)-C(11)	122.91(8)
O(2)-Ta(1)-N(4)	83.93(3)	C(13)-C(12)-C(11)	118.12(9)
N(1)-Ta(1)-N(4)	82.93(3)	C(14)-C(13)-C(12)	121.63(9)
N(2)-Ta(1)-Cl(1)	100.20(3)	C(14)-C(13)-H(13)	121.2(7)
O(1)-Ta(1)-Cl(1)	96.48(2)	C(12)-C(13)-H(13)	117.1(7)
O(2)-Ta(1)-Cl(1)	98.88(2)	C(13)-C(14)-C(15)	117.55(8)
N(1)-Ta(1)-Cl(1)	167.76(2)	C(13)-C(14)-C(26)	123.06(9)
N(4)-Ta(1)-Cl(1)	84.96(2)	C(15)-C(14)-C(26)	119.39(9)
C(1)-O(1)-Ta(1)	122.67(7)	C(16)-C(15)-C(14)	123.50(10)
C(17)-O(2)-Ta(1)	130.68(6)	C(16)-C(15)-H(15)	118.1(6)
C(7)-N(1)-C(11)	119.42(9)	C(14)-C(15)-H(15)	118.3(6)
C(7)-N(1)-Ta(1)	118.11(6)	C(15)-C(16)-C(17)	116.85(9)
C(11)-N(1)-Ta(1)	122.28(7)	C(15)-C(16)-C(30)	121.12(9)
N(3)-N(2)-Ta(1)	174.63(8)	C(17)-C(16)-C(30)	122.03(8)
N(2)-N(3)-C(40)	116.90(9)	O(2)-C(17)-C(12)	118.26(9)
N(2)-N(3)-C(34)	117.37(10)	O(2)-C(17)-C(16)	120.95(9)
C(40)-N(3)-C(34)	123.11(9)	C(12)-C(17)-C(16)	120.78(8)
C(50)-N(4)-C(46)	117.81(9)	C(20)-C(18)-C(2)	111.78(11)
C(50)-N(4)-Ta(1)	120.81(7)	C(20)-C(18)-C(19)	106.96(11)
C(46)-N(4)-Ta(1)	121.32(7)	C(2)-C(18)-C(19)	110.27(9)
O(1)-C(1)-C(6)	118.90(9)	C(20)-C(18)-C(21)	107.72(10)
O(1)-C(1)-C(2)	120.32(10)	C(2)-C(18)-C(21)	110.70(10)
C(6)-C(1)-C(2)	120.77(10)	C(19)-C(18)-C(21)	109.29(11)
C(3)-C(2)-C(1)	116.71(11)	C(18)-C(19)-H(19A)	109.1(9)
C(3)-C(2)-C(18)	122.08(10)	C(18)-C(19)-H(19B)	108.0(7)

H(19A)-C(19)-H(19B)	111.1(13)	H(28A)-C(28)-H(28B)	121.7(13)
C(18)-C(19)-H(19C)	111.6(8)	C(26)-C(28)-H(28C)	109.6(9)
H(19A)-C(19)-H(19C)	108.1(12)	H(28A)-C(28)-H(28C)	102.2(12)
H(19B)-C(19)-H(19C)	109.0(13)	H(28B)-C(28)-H(28C)	112.4(13)
C(18)-C(20)-H(20A)	110.9(10)	C(26)-C(29)-H(29A)	108.9(8)
C(18)-C(20)-H(20B)	110.5(9)	C(26)-C(29)-H(29B)	108.3(8)
H(20A)-C(20)-H(20B)	107.4(12)	H(29A)-C(29)-H(29B)	108.8(11)
C(18)-C(20)-H(20C)	111.5(9)	C(26)-C(29)-H(29C)	110.2(8)
H(20A)-C(20)-H(20C)	109.9(13)	H(29A)-C(29)-H(29C)	109.8(11)
H(20B)-C(20)-H(20C)	106.5(13)	H(29B)-C(29)-H(29C)	110.7(12)
C(18)-C(21)-H(21A)	112.1(8)	C(31)-C(30)-C(32)	107.38(10)
C(18)-C(21)-H(21B)	110.3(8)	C(31)-C(30)-C(33)	107.27(10)
H(21A)-C(21)-H(21B)	109.4(13)	C(32)-C(30)-C(33)	109.58(9)
C(18)-C(21)-H(21C)	111.1(9)	C(31)-C(30)-C(16)	112.02(8)
H(21A)-C(21)-H(21C)	108.6(12)	C(32)-C(30)-C(16)	109.21(9)
H(21B)-C(21)-H(21C)	105.1(11)	C(33)-C(30)-C(16)	111.29(10)
C(23)-C(22)-C(25)	109.68(11)	C(30)-C(31)-H(31A)	111.4(9)
C(23)-C(22)-C(4)	108.90(10)	C(30)-C(31)-H(31B)	111.0(9)
C(25)-C(22)-C(4)	111.40(10)	H(31A)-C(31)-H(31B)	110.6(12)
C(23)-C(22)-C(24)	108.72(13)	C(30)-C(31)-H(31C)	108.4(9)
C(25)-C(22)-C(24)	106.89(11)	H(31A)-C(31)-H(31C)	106.0(13)
C(4)-C(22)-C(24)	111.19(10)	H(31B)-C(31)-H(31C)	109.4(13)
C(22)-C(23)-H(23A)	109.0(10)	C(30)-C(32)-H(32A)	110.1(8)
C(22)-C(23)-H(23B)	109.1(8)	C(30)-C(32)-H(32B)	112.2(8)
H(23A)-C(23)-H(23B)	108.3(13)	H(32A)-C(32)-H(32B)	108.3(10)
C(22)-C(23)-H(23C)	106.0(8)	C(30)-C(32)-H(32C)	109.7(8)
H(23A)-C(23)-H(23C)	115.9(12)	H(32A)-C(32)-H(32C)	106.7(12)
H(23B)-C(23)-H(23C)	108.3(13)	H(32B)-C(32)-H(32C)	109.7(12)
C(22)-C(24)-H(24A)	107.5(11)	C(30)-C(33)-H(33A)	110.3(9)
C(22)-C(24)-H(24B)	110.6(10)	C(30)-C(33)-H(33B)	113.9(8)
H(24A)-C(24)-H(24B)	109.2(13)	H(33A)-C(33)-H(33B)	107.6(12)
C(22)-C(24)-H(24C)	110.1(9)	C(30)-C(33)-H(33C)	108.8(8)
H(24A)-C(24)-H(24C)	115.9(14)	H(33A)-C(33)-H(33C)	109.1(12)
H(24B)-C(24)-H(24C)	103.4(13)	H(33B)-C(33)-H(33C)	106.9(10)
C(22)-C(25)-H(25A)	110.9(8)	C(39)-C(34)-C(35)	119.88(11)
C(22)-C(25)-H(25B)	108.6(9)	C(39)-C(34)-N(3)	120.23(10)
H(25A)-C(25)-H(25B)	110.9(14)	C(35)-C(34)-N(3)	119.89(12)
C(22)-C(25)-H(25C)	110.0(10)	C(34)-C(35)-C(36)	119.33(15)
H(25A)-C(25)-H(25C)	110.0(14)	C(34)-C(35)-H(35)	119.2(9)
H(25B)-C(25)-H(25C)	106.3(12)	C(36)-C(35)-H(35)	121.5(9)
C(28)-C(26)-C(27)	109.66(13)	C(37)-C(36)-C(35)	120.77(14)
C(28)-C(26)-C(29)	108.91(11)	C(37)-C(36)-H(36)	123.4(10)
C(27)-C(26)-C(29)	107.18(11)	C(35)-C(36)-H(36)	115.7(10)
C(28)-C(26)-C(14)	109.70(10)	C(38)-C(37)-C(36)	119.78(12)
C(27)-C(26)-C(14)	109.02(10)	C(38)-C(37)-H(37)	120.6(10)
C(29)-C(26)-C(14)	112.32(9)	C(36)-C(37)-H(37)	119.6(10)
C(26)-C(27)-H(27A)	107.3(9)	C(37)-C(38)-C(39)	120.22(15)
C(26)-C(27)-H(27B)	104.7(12)	C(37)-C(38)-H(38)	119.1(9)
H(27A)-C(27)-H(27B)	106.8(13)	C(39)-C(38)-H(38)	120.7(9)
C(26)-C(27)-H(27C)	111.3(9)	C(34)-C(39)-C(38)	120.01(12)
H(27A)-C(27)-H(27C)	111.8(13)	C(34)-C(39)-H(39)	119.9(8)
H(27B)-C(27)-H(27C)	114.4(14)	C(38)-C(39)-H(39)	120.0(9)
C(26)-C(28)-H(28A)	108.9(9)	C(45)-C(40)-C(41)	118.71(12)
C(26)-C(28)-H(28B)	101.8(11)	C(45)-C(40)-N(3)	121.74(11)

C(41)-C(40)-N(3)	119.50(9)	N(4)-C(46)-C(47)	122.59(11)
C(42)-C(41)-C(40)	120.42(11)	N(4)-C(46)-H(46)	117.7(7)
C(42)-C(41)-H(41)	121.7(9)	C(47)-C(46)-H(46)	119.7(7)
C(40)-C(41)-H(41)	117.9(9)	C(48)-C(47)-C(46)	118.80(11)
C(41)-C(42)-C(43)	120.55(13)	C(48)-C(47)-H(47)	122.5(8)
C(41)-C(42)-H(42)	122.4(10)	C(46)-C(47)-H(47)	118.7(8)
C(43)-C(42)-H(42)	117.0(10)	C(47)-C(48)-C(49)	119.52(11)
C(44)-C(43)-C(42)	118.89(14)	C(47)-C(48)-H(48)	120.6(10)
C(44)-C(43)-H(43)	123.6(9)	C(49)-C(48)-H(48)	119.9(10)
C(42)-C(43)-H(43)	117.5(9)	C(48)-C(49)-C(50)	118.80(13)
C(45)-C(44)-C(43)	121.52(13)	C(48)-C(49)-H(49)	124.5(9)
C(45)-C(44)-H(44)	117.4(12)	C(50)-C(49)-H(49)	116.6(9)
C(43)-C(44)-H(44)	121.0(12)	N(4)-C(50)-C(49)	122.44(11)
C(44)-C(45)-C(40)	119.91(13)	N(4)-C(50)-H(50)	117.2(8)
C(44)-C(45)-H(45)	123.4(8)	C(49)-C(50)-H(50)	120.3(8)
C(40)-C(45)-H(45)	116.7(8)		

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT30 (CCDC 719322). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	105(1)	121(1)	111(1)	-9(1)	34(1)	3(1)
Cl(1)	214(1)	173(1)	193(1)	-21(1)	101(1)	33(1)
O(1)	120(3)	128(4)	163(3)	-11(3)	37(3)	1(3)
O(2)	125(3)	163(4)	121(3)	-16(3)	39(2)	-7(3)
N(1)	118(4)	127(5)	123(3)	-8(3)	38(3)	-12(3)
N(2)	138(4)	142(5)	129(3)	-6(3)	47(3)	7(3)
N(3)	166(4)	171(5)	152(3)	29(3)	12(3)	2(4)
N(4)	140(4)	141(5)	148(3)	-1(3)	54(3)	-2(4)
C(1)	122(4)	147(6)	139(4)	0(3)	43(3)	-1(4)
C(2)	151(5)	158(6)	171(4)	-20(4)	57(4)	-17(4)
C(3)	128(5)	203(6)	204(4)	-36(4)	39(4)	-34(4)
C(4)	122(4)	202(6)	192(4)	-25(4)	48(4)	-16(4)
C(5)	133(5)	155(6)	185(4)	-16(4)	57(4)	4(4)
C(6)	115(4)	147(6)	142(4)	-13(3)	41(3)	-14(4)
C(7)	118(4)	128(5)	140(4)	5(3)	40(3)	5(4)
C(8)	135(5)	187(6)	185(4)	-18(4)	60(4)	13(4)
C(9)	175(5)	173(6)	177(4)	-40(4)	73(4)	16(4)
C(10)	157(5)	162(6)	140(4)	-30(4)	41(4)	-11(4)
C(11)	125(4)	136(6)	121(4)	-2(3)	43(3)	-13(4)
C(12)	115(4)	128(5)	149(4)	-10(3)	38(3)	-5(4)
C(13)	142(5)	145(6)	139(4)	-14(3)	39(3)	-5(4)
C(14)	140(5)	138(6)	156(4)	-6(4)	23(3)	-5(4)
C(15)	120(5)	159(6)	186(4)	-6(4)	32(4)	-10(4)
C(16)	129(4)	135(6)	168(4)	-5(4)	53(3)	-6(4)
C(17)	125(4)	119(5)	136(4)	-5(3)	31(3)	-5(4)
C(18)	183(5)	137(6)	231(5)	-25(4)	47(4)	-28(4)
C(19)	304(7)	161(7)	279(6)	13(5)	89(5)	-15(6)
C(20)	236(6)	189(8)	454(8)	-83(6)	52(6)	-50(6)
C(21)	297(7)	177(7)	265(5)	-63(5)	123(5)	-10(5)
C(22)	114(5)	222(7)	256(5)	-46(4)	36(4)	-4(4)
C(23)	193(6)	477(11)	349(6)	-87(6)	110(5)	22(7)
C(24)	190(6)	309(9)	538(9)	92(7)	24(6)	41(6)
C(25)	177(6)	393(10)	283(6)	-106(6)	-16(5)	48(6)
C(26)	143(5)	225(7)	143(4)	-9(4)	11(3)	-23(4)
C(27)	260(7)	442(10)	240(6)	87(6)	51(5)	106(7)
C(28)	477(10)	381(10)	215(6)	-40(6)	34(6)	-230(8)
C(29)	221(6)	420(10)	168(5)	-3(5)	38(4)	10(6)
C(30)	138(5)	175(6)	190(4)	-16(4)	69(4)	-9(4)
C(31)	161(5)	371(9)	252(5)	-43(5)	99(4)	-54(6)
C(32)	248(6)	179(7)	220(5)	-2(4)	134(5)	-10(5)
C(33)	190(5)	185(7)	246(5)	-13(4)	114(4)	21(5)
C(34)	144(5)	269(7)	134(4)	14(4)	29(4)	7(5)
C(35)	243(6)	371(9)	224(5)	-6(5)	31(5)	107(6)
C(36)	188(6)	623(12)	251(6)	23(6)	-4(5)	139(7)
C(37)	188(6)	605(12)	212(5)	-39(6)	4(5)	-58(6)
C(38)	259(7)	367(9)	209(5)	-45(5)	57(5)	-112(6)
C(39)	177(5)	270(7)	176(4)	11(5)	32(4)	-30(5)

C(40)	207(5)	150(6)	218(5)	23(4)	101(4)	29(5)
C(41)	204(6)	179(7)	262(5)	26(4)	64(4)	-1(5)
C(42)	242(6)	184(7)	428(7)	16(5)	97(6)	-4(5)
C(43)	463(10)	199(8)	599(9)	53(7)	318(8)	-58(7)
C(44)	757(13)	305(9)	384(7)	82(6)	327(8)	-67(9)
C(45)	527(10)	248(8)	232(5)	31(5)	166(6)	-28(7)
C(46)	188(5)	180(6)	179(4)	-18(4)	87(4)	-6(5)
C(47)	311(7)	238(7)	158(4)	-2(4)	108(4)	-27(5)
C(48)	315(7)	422(10)	177(5)	97(5)	39(5)	53(7)
C(49)	184(6)	493(10)	287(6)	147(6)	30(5)	85(6)
C(50)	158(5)	288(8)	210(5)	55(4)	66(4)	27(5)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for IAT30 (CCDC 719322).

	x	y	z	U_{iso}
H(3)	4556(10)	2799(7)	3443(8)	21(3)
H(5)	3611(9)	1033(7)	2259(7)	11(3)
H(8)	2841(9)	857(6)	852(7)	11(3)
H(9)	1775(9)	197(7)	-271(7)	14(3)
H(10)	213(10)	383(7)	-702(8)	25(4)
H(13)	-929(9)	1087(6)	-1452(7)	12(3)
H(15)	-3268(9)	1117(6)	-958(7)	10(3)
H(19A)	2863(11)	3839(8)	1513(9)	35(4)
H(19B)	2395(10)	4325(8)	1962(8)	21(3)
H(19C)	1927(10)	3686(7)	1536(8)	24(4)
H(20A)	4218(11)	3769(8)	3898(9)	35(4)
H(20B)	3789(11)	4390(9)	3331(9)	35(4)
H(20C)	4309(11)	3889(8)	2963(9)	35(4)
H(21A)	1816(11)	3410(8)	3112(8)	28(4)
H(21B)	2298(10)	4087(8)	3455(8)	27(4)
H(21C)	2721(10)	3467(7)	3989(9)	27(4)
H(23A)	5245(12)	1260(9)	2183(10)	53(5)
H(23B)	6279(12)	1309(8)	3009(9)	40(4)
H(23C)	5761(12)	2031(9)	2577(9)	41(5)
H(24A)	4865(13)	892(9)	4257(11)	59(5)
H(24B)	5847(13)	665(9)	4110(10)	50(5)
H(24C)	4861(13)	546(9)	3245(10)	47(5)
H(25A)	5974(12)	2409(9)	4062(9)	41(5)
H(25B)	6392(11)	1728(8)	4602(9)	35(4)
H(25C)	5506(12)	2043(8)	4687(10)	44(5)
H(27A)	-3855(11)	1634(8)	-3382(9)	38(4)
H(27B)	-3138(14)	2042(10)	-2526(11)	58(6)
H(27C)	-3992(12)	1596(9)	-2371(10)	47(5)
H(28A)	-3759(11)	392(8)	-2262(9)	35(4)
H(28B)	-2797(15)	65(11)	-2493(11)	70(6)
H(28C)	-3827(12)	399(8)	-3295(10)	43(4)
H(29A)	-2703(10)	1096(7)	-3691(8)	26(4)
H(29B)	-1824(11)	724(8)	-2887(9)	35(4)
H(29C)	-1877(11)	1578(8)	-2892(9)	38(4)
H(31A)	-3771(11)	696(8)	112(9)	32(4)
H(31B)	-3973(11)	1466(8)	-66(9)	37(4)
H(31C)	-3921(10)	1112(8)	841(9)	32(4)
H(32A)	-2497(10)	734(7)	2049(8)	27(4)
H(32B)	-1549(10)	781(7)	1938(7)	15(3)
H(32C)	-2319(10)	297(8)	1323(8)	29(4)
H(33A)	-2780(11)	2274(8)	904(9)	33(4)
H(33B)	-1885(10)	2068(7)	1698(8)	19(3)
H(33C)	-2833(10)	1932(7)	1762(8)	23(3)
H(35)	3157(10)	572(8)	4553(8)	22(4)
H(36)	4470(12)	950(8)	5699(9)	42(4)
H(37)	4538(13)	2057(8)	6221(10)	47(5)
H(38)	3298(11)	2752(8)	5424(9)	29(4)
H(39)	1954(10)	2357(7)	4216(8)	24(4)

H(41)	402(10)	475(7)	2271(9)	29(4)
H(42)	-400(12)	-494(8)	2409(9)	43(4)
H(43)	-158(11)	-913(8)	3786(9)	34(4)
H(44)	960(14)	-443(10)	5153(12)	68(6)
H(45)	1754(10)	526(8)	5042(9)	29(4)
H(46)	823(9)	2749(6)	178(7)	9(3)
H(47)	128(10)	3309(7)	-1205(8)	27(4)
H(48)	-1485(12)	3585(9)	-1703(10)	55(5)
H(49)	-2267(12)	3257(8)	-732(9)	37(4)
H(50)	-1467(9)	2731(7)	645(8)	19(3)

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 23 July 2008

Crystal Structure Analysis of:

Complex 9 (IAT19)

(shown below)

For Investigator: Ian Tonks ext. 6576

Advisor: J. E. Bercaw ext. 6577

By Michael W. Day 116 Beckman ext. 2734

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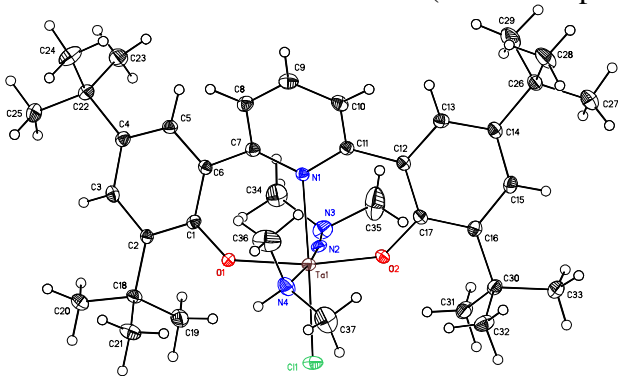
Contents



IAT19

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC). The deposition number is 965847.

Table 1. Crystal data and structure refinement for IAT19 (CCDC 695847).

Empirical formula	$C_{37}H_{56}N_4O_2ClTa$
Formula weight	805.26
Crystallization Solvent	Benzene
Crystal Habit	Block
Crystal size	0.21 x 0.15 x 0.14 mm^3
Crystal color	Yellow

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9943 reflections used in lattice determination	2.49 to 36.04°
Unit cell dimensions	a = 34.7022(12) Å b = 9.2582(3) Å c = 23.1835(9) Å
Volume	7448.4(5) $Å^3$
Z	8
Crystal system	Orthorhombic
Space group	P*bcn*
Density (calculated)	1.436 Mg/m^3
F(000)	3296
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	1.76 to 36.42°
Completeness to θ = 36.42°	95.5 %
Index ranges	$-57 \le h \le 56$, $-15 \le k \le 10$, $-37 \le l \le 36$
Data collection scan type	ω scans; 18 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	288039
Independent reflections	17376 [R_{int}= 0.0612]
Absorption coefficient	3.059 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.6740 and 0.5659

Table 1 (cont.)

Structure solution and Refinement

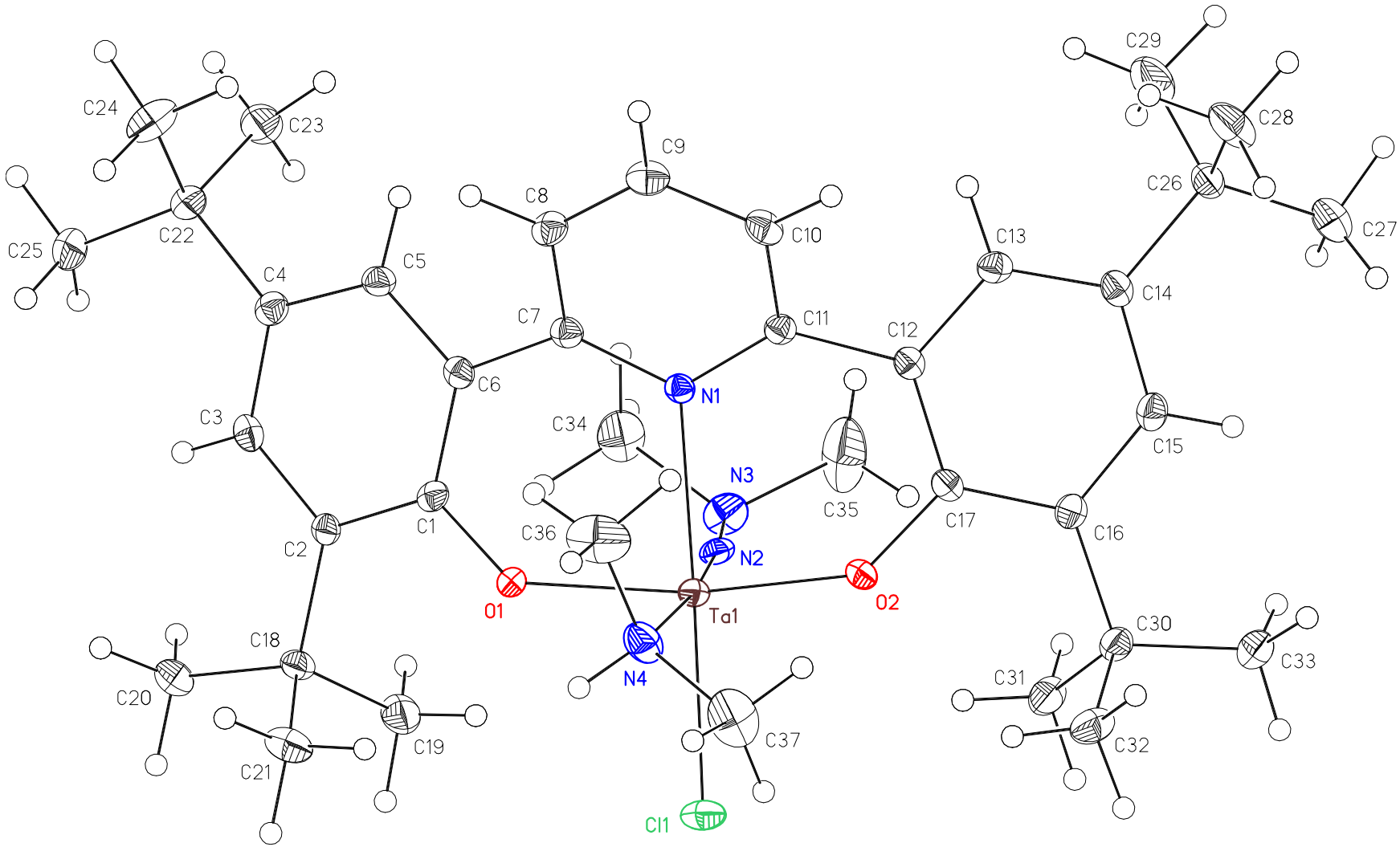
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	17376 / 0 / 630
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.939
Final R indices [$I>2\sigma(I)$, 12465 reflections]	R1 = 0.0401, *w*R2 = 0.0439
R indices (all data)	R1 = 0.0614, *w*R2 = 0.0448
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.004
Average shift/error	0.000
Largest diff. peak and hole	2.791 and -2.460 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C34
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N3
C35
C1
C36
C17
C16
C2
N2
O1
Ta1
O2
C18
N4
C30
C33
C20
C31
C19
C37
C32
C21
Cl1

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT19 (CCDC 695847). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	1496(1)	8726(1)	4987(1)	11(1)
Cl(1)	1829(1)	10865(1)	5309(1)	19(1)
O(1)	1837(1)	8339(1)	4326(1)	13(1)
O(2)	1279(1)	8267(1)	5750(1)	14(1)
N(1)	1287(1)	6419(1)	4788(1)	10(1)
N(2)	1091(1)	9496(1)	4619(1)	13(1)
N(3)	791(1)	10015(1)	4300(1)	20(1)
N(4)	2068(1)	7602(2)	5403(1)	19(1)
C(1)	1758(1)	7772(2)	3803(1)	12(1)
C(2)	1888(1)	8426(2)	3290(1)	11(1)
C(3)	1804(1)	7712(2)	2775(1)	14(1)
C(4)	1595(1)	6427(2)	2741(1)	14(1)
C(5)	1470(1)	5839(2)	3258(1)	13(1)
C(6)	1552(1)	6473(2)	3789(1)	12(1)
C(7)	1422(1)	5699(2)	4316(1)	12(1)
C(8)	1420(1)	4185(2)	4294(1)	15(1)
C(9)	1267(1)	3394(2)	4737(1)	17(1)
C(10)	1097(1)	4127(2)	5188(1)	16(1)
C(11)	1094(1)	5628(2)	5201(1)	12(1)
C(12)	844(1)	6352(2)	5635(1)	11(1)
C(13)	496(1)	5679(2)	5775(1)	14(1)
C(14)	244(1)	6252(2)	6173(1)	14(1)
C(15)	352(1)	7553(2)	6435(1)	15(1)
C(16)	692(1)	8289(2)	6308(1)	13(1)
C(17)	939(1)	7665(2)	5897(1)	12(1)
C(18)	2107(1)	9874(2)	3296(1)	15(1)
C(19)	1839(1)	11062(2)	3531(1)	22(1)
C(20)	2230(1)	10340(2)	2686(1)	22(1)
C(21)	2471(1)	9780(2)	3664(1)	23(1)
C(22)	1491(1)	5671(2)	2173(1)	17(1)
C(23)	1052(1)	5697(2)	2098(1)	22(1)
C(24)	1624(1)	4096(2)	2194(1)	28(1)
C(25)	1678(1)	6389(2)	1652(1)	25(1)
C(26)	-131(1)	5462(2)	6322(1)	17(1)
C(27)	-399(1)	6373(2)	6693(1)	30(1)
C(28)	-31(1)	4068(2)	6651(1)	28(1)
C(29)	-347(1)	5063(3)	5770(1)	30(1)
C(30)	784(1)	9737(2)	6603(1)	15(1)
C(31)	790(1)	10937(2)	6140(1)	19(1)
C(32)	1174(1)	9661(2)	6911(1)	21(1)
C(33)	481(1)	10156(2)	7051(1)	23(1)
C(34)	792(1)	9424(2)	3717(1)	28(1)
C(35)	423(1)	9797(4)	4588(1)	44(1)
C(36)	2121(1)	6050(2)	5283(1)	32(1)
C(37)	2154(1)	7913(3)	6014(1)	31(1)

Table 3. Selected bond lengths [Å] and angles [°] for IAT19 (CCDC 695847).

Ta(1)-N(2)	1.7890(14)	N(2)-Ta(1)-O(2)	102.42(6)
Ta(1)-O(2)	1.9677(12)	N(2)-Ta(1)-O(1)	99.98(6)
Ta(1)-O(1)	1.9696(11)	O(2)-Ta(1)-O(1)	152.78(5)
Ta(1)-N(1)	2.3026(12)	N(2)-Ta(1)-N(1)	91.57(5)
Ta(1)-Cl(1)	2.4109(4)	O(2)-Ta(1)-N(1)	81.92(5)
Ta(1)-N(4)	2.4425(15)	O(1)-Ta(1)-N(1)	82.20(4)
		N(2)-Ta(1)-Cl(1)	101.32(4)
		O(2)-Ta(1)-Cl(1)	94.71(3)
		O(1)-Ta(1)-Cl(1)	95.88(3)
		N(1)-Ta(1)-Cl(1)	167.10(3)
		N(2)-Ta(1)-N(4)	174.82(6)
		O(2)-Ta(1)-N(4)	82.11(5)
		O(1)-Ta(1)-N(4)	74.99(5)
		N(1)-Ta(1)-N(4)	86.55(5)
		Cl(1)-Ta(1)-N(4)	80.64(4)

Table 4. Bond lengths [Å] and angles [°] for IAT19 (CCDC 695847).

Ta(1)-N(2)	1.7890(14)	C(20)-H(20A)	0.979(18)
Ta(1)-O(2)	1.9677(12)	C(20)-H(20B)	0.96(2)
Ta(1)-O(1)	1.9696(11)	C(20)-H(20C)	1.00(2)
Ta(1)-N(1)	2.3026(12)	C(21)-H(21A)	0.915(19)
Ta(1)-Cl(1)	2.4109(4)	C(21)-H(21B)	0.984(19)
Ta(1)-N(4)	2.4425(15)	C(21)-H(21C)	0.997(19)
O(1)-C(1)	1.3489(19)	C(22)-C(25)	1.523(3)
O(2)-C(17)	1.3488(19)	C(22)-C(24)	1.530(3)
N(1)-C(7)	1.364(2)	C(22)-C(23)	1.535(3)
N(1)-C(11)	1.378(2)	C(23)-H(23A)	0.954(19)
N(2)-N(3)	1.3651(19)	C(23)-H(23B)	0.925(18)
N(3)-C(35)	1.455(3)	C(23)-H(23C)	0.92(2)
N(3)-C(34)	1.459(3)	C(24)-H(24A)	1.02(2)
N(4)-C(37)	1.475(3)	C(24)-H(24B)	0.98(2)
N(4)-C(36)	1.475(2)	C(24)-H(24C)	0.96(2)
N(4)-H(4)	0.85(2)	C(25)-H(25A)	1.01(2)
C(1)-C(6)	1.399(2)	C(25)-H(25B)	0.93(2)
C(1)-C(2)	1.410(2)	C(25)-H(25C)	0.990(18)
C(2)-C(3)	1.395(2)	C(26)-C(27)	1.525(3)
C(2)-C(18)	1.541(2)	C(26)-C(29)	1.529(3)
C(3)-C(4)	1.395(2)	C(26)-C(28)	1.539(3)
C(3)-H(3)	0.872(16)	C(27)-H(27A)	0.95(2)
C(4)-C(5)	1.386(2)	C(27)-H(27B)	0.97(2)
C(4)-C(22)	1.536(2)	C(27)-H(27C)	0.941(19)
C(5)-C(6)	1.394(2)	C(28)-H(28A)	1.02(2)
C(5)-H(5)	0.951(15)	C(28)-H(28B)	0.91(2)
C(6)-C(7)	1.486(2)	C(28)-H(28C)	1.02(2)
C(7)-C(8)	1.403(2)	C(29)-H(29A)	0.927(19)
C(8)-C(9)	1.369(2)	C(29)-H(29B)	0.978(19)
C(8)-H(8)	0.930(16)	C(29)-H(29C)	0.98(2)
C(9)-C(10)	1.377(3)	C(30)-C(33)	1.530(3)
C(9)-H(9)	0.917(17)	C(30)-C(32)	1.530(3)
C(10)-C(11)	1.390(2)	C(30)-C(31)	1.544(2)
C(10)-H(10)	0.888(17)	C(31)-H(31A)	0.962(17)
C(11)-C(12)	1.488(2)	C(31)-H(31B)	0.957(19)
C(12)-C(13)	1.397(2)	C(31)-H(31C)	0.919(19)
C(12)-C(17)	1.399(2)	C(32)-H(32A)	0.960(17)
C(13)-C(14)	1.379(2)	C(32)-H(32B)	0.89(2)
C(13)-H(13)	0.932(15)	C(32)-H(32C)	0.935(18)
C(14)-C(15)	1.401(2)	C(33)-H(33A)	0.982(18)
C(14)-C(26)	1.530(2)	C(33)-H(33B)	0.92(2)
C(15)-C(16)	1.393(2)	C(33)-H(33C)	0.913(18)
C(15)-H(15)	0.914(15)	C(34)-H(34A)	1.00(2)
C(16)-C(17)	1.407(2)	C(34)-H(34B)	1.07(2)
C(16)-C(30)	1.539(2)	C(34)-H(34C)	1.04(2)
C(18)-C(21)	1.526(3)	C(35)-H(35A)	0.99(2)
C(18)-C(20)	1.538(3)	C(35)-H(35B)	0.94(3)
C(18)-C(19)	1.541(2)	C(35)-H(35C)	0.87(3)
C(19)-H(19A)	0.91(2)	C(36)-H(36A)	0.97(2)
C(19)-H(19B)	0.94(2)	C(36)-H(36B)	0.94(2)
C(19)-H(19C)	0.981(17)	C(36)-H(36C)	1.00(2)

C(37)-H(37A)	0.93(2)	C(8)-C(7)-C(6)	117.00(15)
C(37)-H(37B)	1.018(18)	C(9)-C(8)-C(7)	120.60(16)
C(37)-H(37C)	0.99(2)	C(9)-C(8)-H(8)	121.5(9)
		C(7)-C(8)-H(8)	117.9(9)
N(2)-Ta(1)-O(2)	102.42(6)	C(8)-C(9)-C(10)	118.15(15)
N(2)-Ta(1)-O(1)	99.98(6)	C(8)-C(9)-H(9)	122.3(12)
O(2)-Ta(1)-O(1)	152.78(5)	C(10)-C(9)-H(9)	119.5(12)
N(2)-Ta(1)-N(1)	91.57(5)	C(9)-C(10)-C(11)	120.77(16)
O(2)-Ta(1)-N(1)	81.92(5)	C(9)-C(10)-H(10)	121.4(11)
O(1)-Ta(1)-N(1)	82.20(4)	C(11)-C(10)-H(10)	117.8(11)
N(2)-Ta(1)-Cl(1)	101.32(4)	N(1)-C(11)-C(10)	120.84(15)
O(2)-Ta(1)-Cl(1)	94.71(3)	N(1)-C(11)-C(12)	120.89(13)
O(1)-Ta(1)-Cl(1)	95.88(3)	C(10)-C(11)-C(12)	117.95(15)
N(1)-Ta(1)-Cl(1)	167.10(3)	C(13)-C(12)-C(17)	119.36(15)
N(2)-Ta(1)-N(4)	174.82(6)	C(13)-C(12)-C(11)	117.44(14)
O(2)-Ta(1)-N(4)	82.11(5)	C(17)-C(12)-C(11)	123.19(14)
O(1)-Ta(1)-N(4)	74.99(5)	C(14)-C(13)-C(12)	122.25(15)
N(1)-Ta(1)-N(4)	86.55(5)	C(14)-C(13)-H(13)	119.5(11)
Cl(1)-Ta(1)-N(4)	80.64(4)	C(12)-C(13)-H(13)	118.3(11)
C(1)-O(1)-Ta(1)	130.37(10)	C(13)-C(14)-C(15)	116.78(15)
C(17)-O(2)-Ta(1)	130.64(11)	C(13)-C(14)-C(26)	120.45(15)
C(7)-N(1)-C(11)	117.67(12)	C(15)-C(14)-C(26)	122.76(15)
C(7)-N(1)-Ta(1)	120.40(10)	C(16)-C(15)-C(14)	123.75(16)
C(11)-N(1)-Ta(1)	120.39(10)	C(16)-C(15)-H(15)	118.8(9)
N(3)-N(2)-Ta(1)	175.26(12)	C(14)-C(15)-H(15)	117.4(9)
N(2)-N(3)-C(35)	111.87(17)	C(15)-C(16)-C(17)	117.40(14)
N(2)-N(3)-C(34)	111.66(14)	C(15)-C(16)-C(30)	120.59(15)
C(35)-N(3)-C(34)	111.96(18)	C(17)-C(16)-C(30)	122.01(15)
C(37)-N(4)-C(36)	110.30(17)	O(2)-C(17)-C(12)	117.04(14)
C(37)-N(4)-Ta(1)	117.42(12)	O(2)-C(17)-C(16)	122.50(14)
C(36)-N(4)-Ta(1)	116.11(12)	C(12)-C(17)-C(16)	120.44(15)
C(37)-N(4)-H(4)	106.8(14)	C(21)-C(18)-C(2)	111.31(14)
C(36)-N(4)-H(4)	104.4(14)	C(21)-C(18)-C(20)	107.51(16)
Ta(1)-N(4)-H(4)	99.9(15)	C(2)-C(18)-C(20)	111.82(14)
O(1)-C(1)-C(6)	117.32(15)	C(21)-C(18)-C(19)	110.02(16)
O(1)-C(1)-C(2)	121.72(14)	C(2)-C(18)-C(19)	109.08(14)
C(6)-C(1)-C(2)	120.92(15)	C(20)-C(18)-C(19)	107.01(15)
C(3)-C(2)-C(1)	116.83(14)	C(18)-C(19)-H(19A)	112.0(12)
C(3)-C(2)-C(18)	121.59(15)	C(18)-C(19)-H(19B)	110.3(12)
C(1)-C(2)-C(18)	121.57(15)	H(19A)-C(19)-H(19B)	109.3(18)
C(2)-C(3)-C(4)	124.08(16)	C(18)-C(19)-H(19C)	110.4(11)
C(2)-C(3)-H(3)	117.6(11)	H(19A)-C(19)-H(19C)	103.6(15)
C(4)-C(3)-H(3)	118.2(11)	H(19B)-C(19)-H(19C)	111.0(15)
C(5)-C(4)-C(3)	116.76(16)	C(18)-C(20)-H(20A)	110.3(12)
C(5)-C(4)-C(22)	119.26(15)	C(18)-C(20)-H(20B)	111.5(12)
C(3)-C(4)-C(22)	123.97(16)	H(20A)-C(20)-H(20B)	108.3(15)
C(4)-C(5)-C(6)	122.25(15)	C(18)-C(20)-H(20C)	113.2(11)
C(4)-C(5)-H(5)	118.7(10)	H(20A)-C(20)-H(20C)	104.4(17)
C(6)-C(5)-H(5)	119.0(10)	H(20B)-C(20)-H(20C)	108.8(16)
C(5)-C(6)-C(1)	119.13(15)	C(18)-C(21)-H(21A)	110.0(13)
C(5)-C(6)-C(7)	117.43(14)	C(18)-C(21)-H(21B)	115.4(12)
C(1)-C(6)-C(7)	123.42(15)	H(21A)-C(21)-H(21B)	108.4(16)
N(1)-C(7)-C(8)	121.05(15)	C(18)-C(21)-H(21C)	112.4(11)
N(1)-C(7)-C(6)	121.82(13)	H(21A)-C(21)-H(21C)	106.3(17)

H(21B)-C(21)-H(21C)	103.8(15)	C(33)-C(30)-C(32)	107.65(16)
C(25)-C(22)-C(24)	108.27(17)	C(33)-C(30)-C(16)	112.25(14)
C(25)-C(22)-C(23)	109.13(16)	C(32)-C(30)-C(16)	110.62(14)
C(24)-C(22)-C(23)	108.55(16)	C(33)-C(30)-C(31)	107.33(15)
C(25)-C(22)-C(4)	112.35(15)	C(32)-C(30)-C(31)	110.21(15)
C(24)-C(22)-C(4)	109.65(15)	C(16)-C(30)-C(31)	108.73(14)
C(23)-C(22)-C(4)	108.82(15)	C(30)-C(31)-H(31A)	109.1(11)
C(22)-C(23)-H(23A)	113.3(13)	C(30)-C(31)-H(31B)	110.1(10)
C(22)-C(23)-H(23B)	109.4(12)	H(31A)-C(31)-H(31B)	111.1(14)
H(23A)-C(23)-H(23B)	111.2(16)	C(30)-C(31)-H(31C)	112.9(11)
C(22)-C(23)-H(23C)	112.0(13)	H(31A)-C(31)-H(31C)	106.2(15)
H(23A)-C(23)-H(23C)	106.8(16)	H(31B)-C(31)-H(31C)	107.4(15)
H(23B)-C(23)-H(23C)	103.7(15)	C(30)-C(32)-H(32A)	110.7(11)
C(22)-C(24)-H(24A)	112.5(12)	C(30)-C(32)-H(32B)	115.2(13)
C(22)-C(24)-H(24B)	109.1(11)	H(32A)-C(32)-H(32B)	104.9(16)
H(24A)-C(24)-H(24B)	106.6(17)	C(30)-C(32)-H(32C)	110.1(12)
C(22)-C(24)-H(24C)	109.2(12)	H(32A)-C(32)-H(32C)	105.9(15)
H(24A)-C(24)-H(24C)	107.6(17)	H(32B)-C(32)-H(32C)	109.6(16)
H(24B)-C(24)-H(24C)	111.8(17)	C(30)-C(33)-H(33A)	113.2(11)
C(22)-C(25)-H(25A)	109.8(11)	C(30)-C(33)-H(33B)	112.5(13)
C(22)-C(25)-H(25B)	110.0(13)	H(33A)-C(33)-H(33B)	106.1(17)
H(25A)-C(25)-H(25B)	109.7(17)	C(30)-C(33)-H(33C)	109.9(12)
C(22)-C(25)-H(25C)	117.9(11)	H(33A)-C(33)-H(33C)	105.7(16)
H(25A)-C(25)-H(25C)	104.4(15)	H(33B)-C(33)-H(33C)	109.1(16)
H(25B)-C(25)-H(25C)	104.7(16)	N(3)-C(34)-H(34A)	107.8(13)
C(27)-C(26)-C(29)	107.77(17)	N(3)-C(34)-H(34B)	110.6(10)
C(27)-C(26)-C(14)	112.47(14)	H(34A)-C(34)-H(34B)	108.7(16)
C(29)-C(26)-C(14)	110.14(15)	N(3)-C(34)-H(34C)	111.2(13)
C(27)-C(26)-C(28)	108.79(17)	H(34A)-C(34)-H(34C)	112.5(17)
C(29)-C(26)-C(28)	108.86(16)	H(34B)-C(34)-H(34C)	106.0(16)
C(14)-C(26)-C(28)	108.75(15)	N(3)-C(35)-H(35A)	111.2(15)
C(26)-C(27)-H(27A)	114.0(13)	N(3)-C(35)-H(35B)	106.9(16)
C(26)-C(27)-H(27B)	107.9(12)	H(35A)-C(35)-H(35B)	113(2)
H(27A)-C(27)-H(27B)	107.1(18)	N(3)-C(35)-H(35C)	114(2)
C(26)-C(27)-H(27C)	108.6(13)	H(35A)-C(35)-H(35C)	98(2)
H(27A)-C(27)-H(27C)	108.7(16)	H(35B)-C(35)-H(35C)	113(2)
H(27B)-C(27)-H(27C)	110.6(17)	N(4)-C(36)-H(36A)	114.7(12)
C(26)-C(28)-H(28A)	108.5(12)	N(4)-C(36)-H(36B)	113.7(13)
C(26)-C(28)-H(28B)	112.6(12)	H(36A)-C(36)-H(36B)	107.1(19)
H(28A)-C(28)-H(28B)	110.1(16)	N(4)-C(36)-H(36C)	107.3(11)
C(26)-C(28)-H(28C)	113.9(11)	H(36A)-C(36)-H(36C)	107.1(16)
H(28A)-C(28)-H(28C)	104.9(17)	H(36B)-C(36)-H(36C)	106.5(18)
H(28B)-C(28)-H(28C)	106.5(16)	N(4)-C(37)-H(37A)	106.6(14)
C(26)-C(29)-H(29A)	108.4(13)	N(4)-C(37)-H(37B)	111.8(11)
C(26)-C(29)-H(29B)	108.8(11)	H(37A)-C(37)-H(37B)	107.0(18)
H(29A)-C(29)-H(29B)	106.7(17)	N(4)-C(37)-H(37C)	106.6(12)
C(26)-C(29)-H(29C)	111.6(12)	H(37A)-C(37)-H(37C)	110.6(17)
H(29A)-C(29)-H(29C)	108.3(17)	H(37B)-C(37)-H(37C)	114.1(17)
H(29B)-C(29)-H(29C)	112.8(16)		

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for IAT19 (CCDC 695847). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	108(1)	112(1)	123(1)	-12(1)	-3(1)	-14(1)
Cl(1)	178(2)	159(2)	235(2)	-38(2)	-43(2)	-41(2)
O(1)	131(6)	135(5)	113(6)	-29(4)	16(5)	-22(4)
O(2)	112(6)	157(5)	135(6)	-11(5)	11(5)	-39(4)
N(1)	89(6)	109(6)	116(6)	-2(5)	-3(5)	1(5)
N(2)	157(7)	92(6)	133(8)	-26(5)	-9(6)	-18(5)
N(3)	167(8)	221(7)	216(9)	-23(6)	-53(7)	36(6)
N(4)	138(8)	246(8)	198(9)	25(7)	-3(7)	-19(6)
C(1)	97(7)	109(7)	144(9)	-27(6)	-5(6)	27(5)
C(2)	91(7)	114(7)	138(8)	-9(6)	15(6)	14(5)
C(3)	122(8)	143(7)	146(9)	21(7)	29(7)	16(6)
C(4)	126(8)	137(8)	148(9)	-17(7)	-1(6)	18(6)
C(5)	131(8)	107(6)	165(9)	-13(6)	8(7)	-9(6)
C(6)	90(8)	111(7)	150(8)	1(6)	9(6)	19(5)
C(7)	104(8)	123(7)	144(9)	-3(6)	-6(6)	4(5)
C(8)	152(9)	120(7)	180(9)	-21(7)	2(7)	27(6)
C(9)	177(9)	119(7)	213(10)	13(7)	-36(8)	12(6)
C(10)	176(9)	138(7)	154(9)	54(6)	-3(7)	-22(6)
C(11)	121(8)	124(7)	110(8)	4(6)	-11(6)	-7(6)
C(12)	117(7)	130(7)	94(7)	27(6)	-12(6)	-1(6)
C(13)	152(8)	137(7)	115(8)	9(6)	-25(7)	-15(6)
C(14)	122(7)	187(7)	107(8)	30(7)	-11(6)	-12(6)
C(15)	148(8)	187(8)	111(9)	-2(7)	4(7)	15(6)
C(16)	147(8)	146(7)	102(8)	10(6)	-8(7)	7(6)
C(17)	106(8)	151(7)	102(8)	25(6)	-17(6)	-15(6)
C(18)	141(8)	114(7)	187(10)	-9(6)	25(7)	-27(6)
C(19)	235(10)	129(8)	282(12)	2(8)	75(9)	-4(7)
C(20)	252(11)	186(9)	228(11)	4(8)	65(9)	-79(8)
C(21)	180(10)	216(10)	299(13)	5(9)	-18(8)	-64(7)
C(22)	185(9)	173(7)	140(9)	-24(6)	0(7)	-23(7)
C(23)	209(10)	280(10)	166(10)	0(8)	-28(8)	-53(8)
C(24)	370(13)	213(10)	256(12)	-92(9)	-38(10)	28(9)
C(25)	263(11)	329(11)	151(10)	-61(9)	45(8)	-70(9)
C(26)	145(9)	233(9)	134(9)	-4(7)	9(7)	-54(7)
C(27)	188(10)	349(11)	349(13)	-61(11)	96(9)	-78(9)
C(28)	231(11)	316(11)	291(13)	85(9)	26(9)	-97(8)
C(29)	177(10)	521(14)	212(12)	3(10)	-25(9)	-125(10)
C(30)	191(9)	145(7)	122(9)	-11(6)	10(7)	-14(6)
C(31)	246(10)	164(8)	154(10)	-19(7)	13(8)	6(7)
C(32)	254(11)	192(9)	177(11)	-33(8)	-45(8)	-21(7)
C(33)	288(11)	203(9)	204(11)	-60(8)	66(9)	-39(8)
C(34)	227(11)	398(12)	204(12)	16(9)	-62(9)	10(9)
C(35)	179(12)	890(20)	255(14)	-58(14)	-33(10)	137(12)
C(36)	179(10)	269(11)	521(16)	1(11)	-126(11)	69(8)
C(37)	234(12)	468(14)	230(12)	104(10)	-74(10)	18(10)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for IAT19 (CCDC 695847).

	x	y	z	U_{iso}
H(4)	2243(7)	8020(20)	5204(9)	36(6)
H(3)	1879(5)	8114(16)	2454(7)	9(4)
H(5)	1315(5)	4993(16)	3248(7)	6(4)
H(8)	1525(5)	3742(15)	3970(7)	6(4)
H(9)	1269(6)	2404(19)	4739(8)	25(5)
H(10)	986(5)	3661(16)	5478(8)	16(5)
H(13)	435(5)	4816(16)	5589(7)	12(5)
H(15)	183(5)	7953(15)	6693(7)	0(4)
H(19A)	1770(6)	10896(19)	3904(9)	27(6)
H(19B)	1616(6)	11132(18)	3303(9)	25(6)
H(19C)	1975(5)	11989(18)	3548(8)	21(5)
H(20A)	2379(6)	11238(19)	2703(9)	30(6)
H(20B)	2011(6)	10495(18)	2441(8)	21(6)
H(20C)	2408(7)	9632(18)	2495(8)	31(6)
H(21A)	2635(6)	9107(19)	3514(8)	25(6)
H(21B)	2428(6)	9550(19)	4074(9)	24(6)
H(21C)	2616(6)	10710(20)	3675(8)	28(5)
H(23A)	945(6)	6650(20)	2114(8)	32(6)
H(23B)	939(6)	5100(17)	2370(8)	15(5)
H(23C)	976(6)	5304(18)	1753(9)	23(5)
H(24A)	1512(6)	3550(20)	2537(11)	44(7)
H(24B)	1905(6)	4068(19)	2238(9)	29(6)
H(24C)	1541(6)	3612(19)	1850(10)	31(6)
H(25A)	1608(6)	5840(20)	1288(9)	32(6)
H(25B)	1944(6)	6400(19)	1696(9)	32(6)
H(25C)	1609(6)	7400(20)	1568(8)	28(6)
H(27A)	-297(7)	6610(20)	7062(9)	38(7)
H(27B)	-633(7)	5820(20)	6758(9)	38(6)
H(27C)	-455(6)	7240(20)	6495(9)	34(6)
H(28A)	139(7)	3440(20)	6393(10)	42(7)
H(28B)	-243(6)	3568(18)	6761(8)	24(5)
H(28C)	128(6)	4230(20)	7014(9)	33(6)
H(29A)	-401(6)	5900(20)	5569(9)	33(6)
H(29B)	-595(6)	4636(18)	5875(8)	23(5)
H(29C)	-193(6)	4433(19)	5520(9)	32(6)
H(31A)	850(5)	11844(18)	6322(8)	20(5)
H(31B)	547(6)	10979(16)	5946(8)	15(5)
H(31C)	976(5)	10794(17)	5865(8)	17(5)
H(32A)	1227(5)	10550(18)	7109(8)	16(5)
H(32B)	1377(6)	9521(18)	6681(8)	21(5)
H(32C)	1168(5)	8946(18)	7195(8)	20(5)
H(33A)	455(6)	9447(19)	7363(8)	27(5)
H(33B)	239(6)	10255(18)	6893(8)	23(6)
H(33C)	549(6)	11003(19)	7225(8)	25(5)
H(34A)	1042(7)	9700(20)	3529(10)	46(7)
H(34B)	560(6)	9865(19)	3470(8)	32(6)
H(34C)	748(7)	8310(20)	3721(10)	59(8)
H(35A)	370(7)	8760(20)	4647(10)	55(8)

H(35B)	234(8)	10270(20)	4362(11)	56(8)
H(35C)	423(9)	10070(30)	4947(12)	78(10)
H(36A)	2362(6)	5650(20)	5418(9)	34(6)
H(36B)	2099(7)	5810(20)	4891(9)	35(7)
H(36C)	1908(7)	5520(20)	5488(9)	35(6)
H(37A)	1968(7)	7430(20)	6231(10)	49(7)
H(37B)	2127(6)	8980(20)	6105(8)	30(6)
H(37C)	2413(7)	7515(19)	6092(9)	35(6)

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 27 October 2009

Crystal Structure Analysis of:

Complex 10 (IAT41)

(shown below)

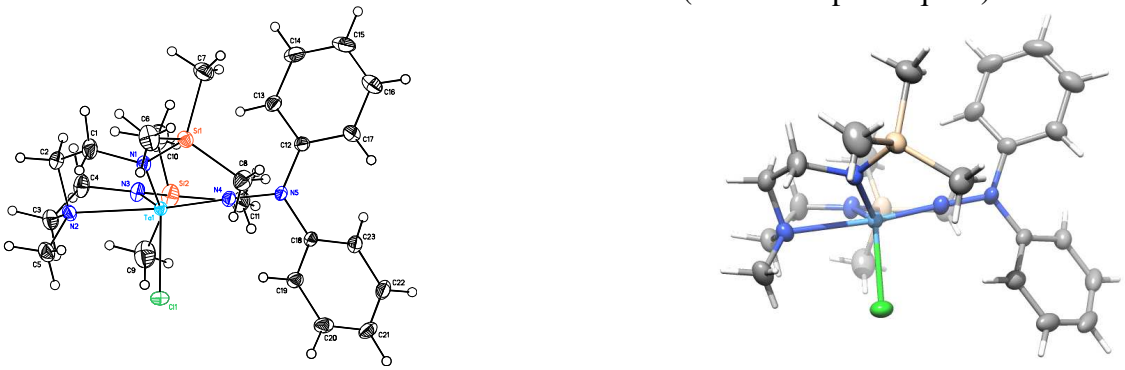
For Investigator: Ian Tonks ext. 6576

Advisor: J. E. Bercaw ext. 6577

By Michael W. Day 116 Beckman ext. 2734

e-mail: mikeday@caltech.edu

Contents

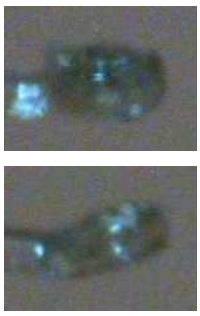


IAT41

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC). The deposition number is 752439.

Table 1. Crystal data and structure refinement for IAT41 (CCDC 752439).

Empirical formula	$C_{23}H_{39}N_5Si_2ClTa$
Formula weight	658.17
Crystallization Solvent	Hexanes/TMS_2O
Crystal Habit	Column
Crystal size	0.23 x 0.14 x 0.08 mm^3
Crystal color	Yellow



Data Collection

Type of diffractometer	Bruker KAPPA APEX II	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 9392 reflections used in lattice determination	2.51 to 40.07°	
Unit cell dimensions	a = 13.1052(6) Å b = 12.9574(6) Å c = 16.9529(8) Å	β= 90.622(3)°
Volume	2878.6(2) $Å^3$	
Z	4	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Density (calculated)	1.519 Mg/m^3	
F(000)	1320	
Data collection program	Bruker APEX2 v2009.7-0	
θ range for data collection	1.95 to 43.76°	
Completeness to θ = 43.76°	98.6 %	
Index ranges	$-25 \le h \le 25$, $-24 \le k \le 25$, $-32 \le l \le 32$	
Data collection scan type	ω scans; 21 settings	
Data reduction program	Bruker SAINT-Plus v7.66A	
Reflections collected	201289	
Independent reflections	21919 [R_{int}= 0.0416]	
Absorption coefficient	4.014 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7486 and 0.5883	

Table 1 (cont.)

Structure solution and Refinement

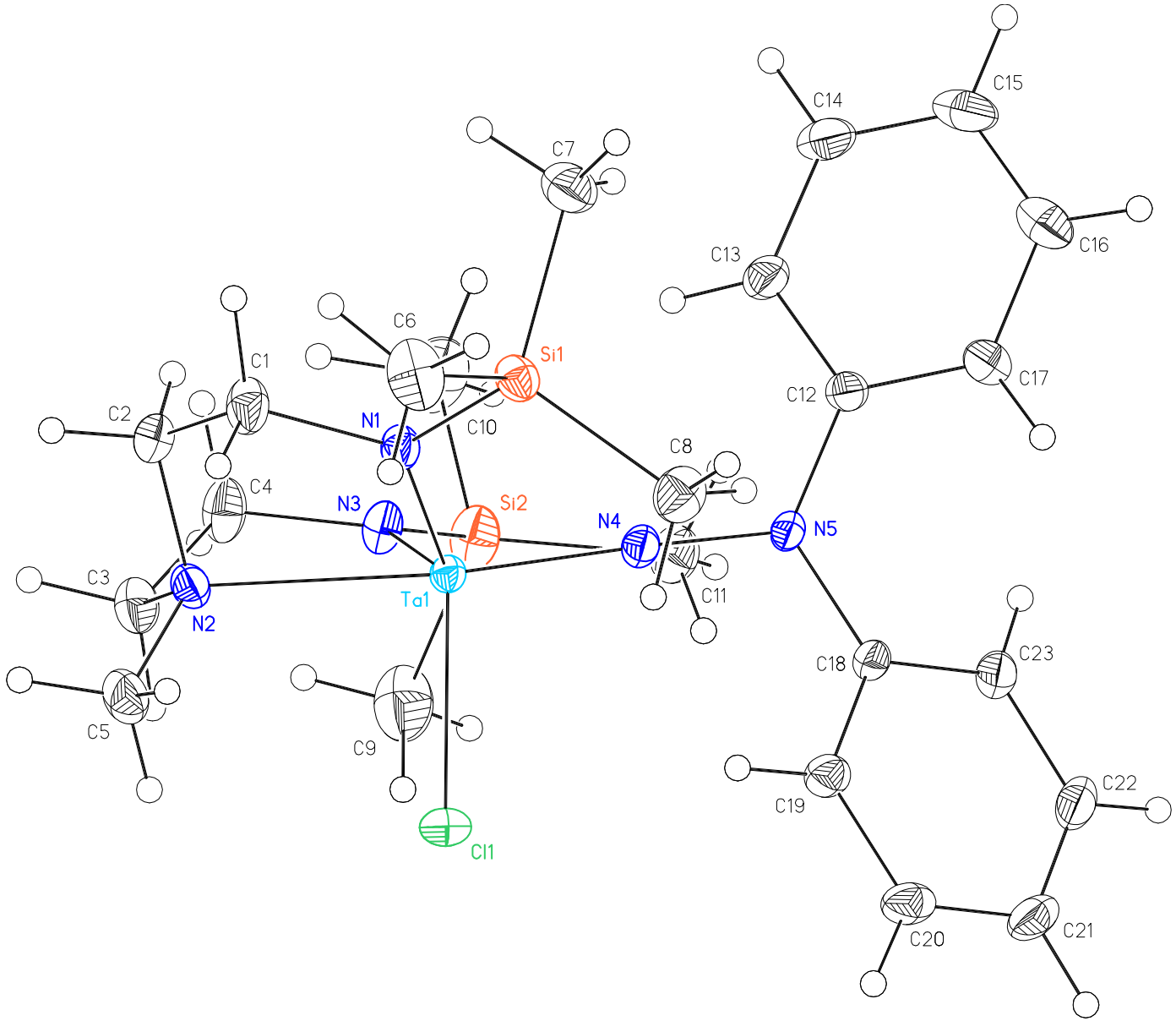
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	21919 / 0 / 445
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	2.205
Final R indices [$I>2\sigma(I)$, 17487 reflections]	R1 = 0.0285, *w*R2 = 0.0506
R indices (all data)	R1 = 0.0444, *w*R2 = 0.0517
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.011
Average shift/error	0.000
Largest diff. peak and hole	4.170 and -2.602 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C16
C13
C6
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C8
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Si2
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C22
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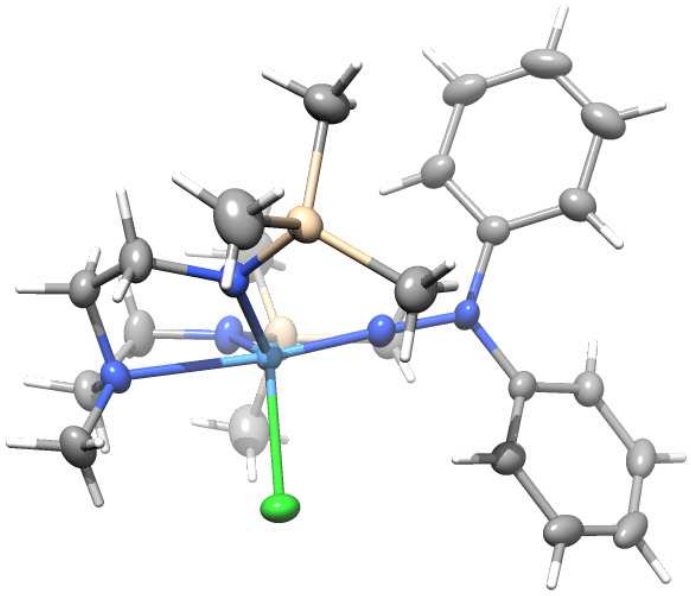
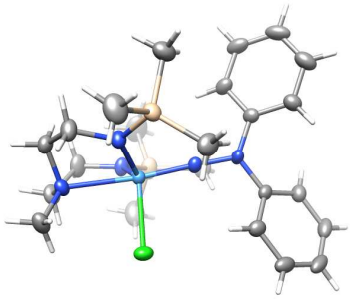
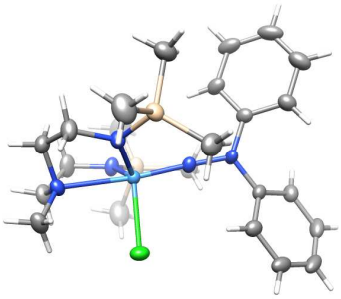
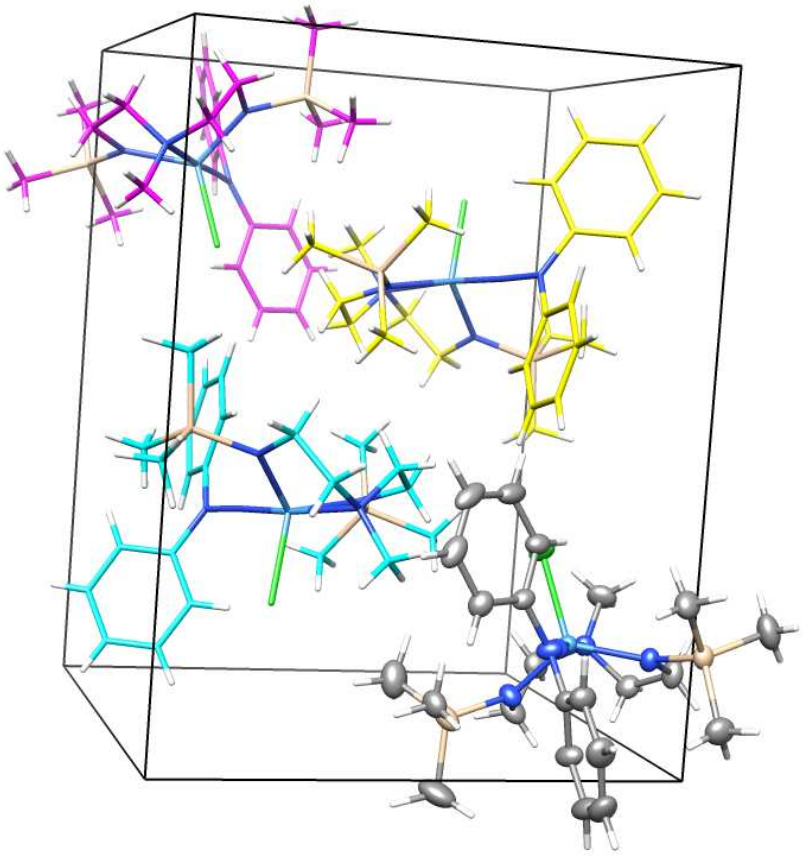
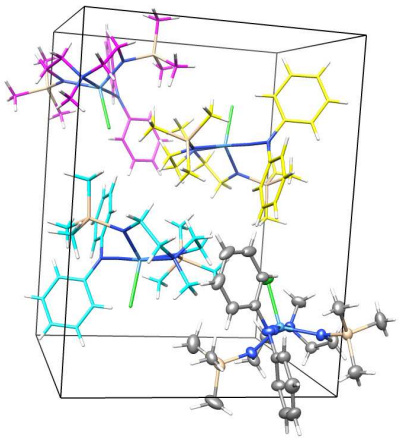
C21











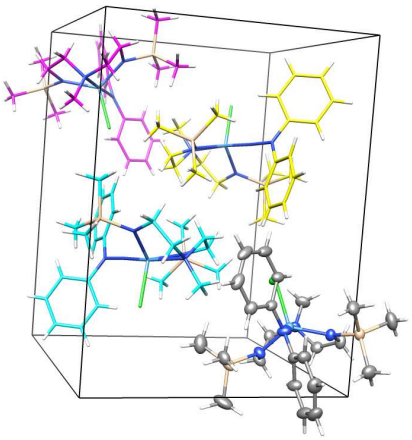


Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT41 (CCDC 752439). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	8572(1)	1893(1)	8278(1)	12(1)
Cl(1)	7856(1)	2282(1)	7029(1)	22(1)
Si(1)	10254(1)	-102(1)	8194(1)	18(1)
Si(2)	8052(1)	3987(1)	9452(1)	25(1)
N(1)	9058(1)	433(1)	8415(1)	17(1)
N(2)	7052(1)	946(1)	8510(1)	17(1)
N(3)	7896(1)	2701(1)	9145(1)	19(1)
N(4)	9771(1)	2548(1)	8183(1)	15(1)
N(5)	10676(1)	3045(1)	8076(1)	16(1)
C(1)	8352(1)	-362(1)	8716(1)	23(1)
C(2)	7419(1)	133(1)	9061(1)	21(1)
C(3)	6353(1)	1660(1)	8916(1)	23(1)
C(4)	6952(1)	2287(1)	9512(1)	25(1)
C(5)	6528(1)	462(1)	7830(1)	25(1)
C(6)	10046(2)	-1459(1)	7842(1)	32(1)
C(7)	11066(1)	-164(1)	9098(1)	28(1)
C(8)	10909(1)	590(1)	7383(1)	25(1)
C(9)	6900(2)	4718(2)	9081(2)	39(1)
C(10)	8089(2)	4076(2)	10548(1)	43(1)
C(11)	9213(1)	4620(1)	9070(1)	24(1)
C(12)	11441(1)	2951(1)	8652(1)	16(1)
C(13)	11194(1)	2718(1)	9433(1)	21(1)
C(14)	11961(1)	2634(1)	10001(1)	26(1)
C(15)	12980(1)	2750(1)	9803(1)	29(1)
C(16)	13227(1)	2963(1)	9028(1)	27(1)
C(17)	12473(1)	3060(1)	8452(1)	21(1)
C(18)	10775(1)	3639(1)	7380(1)	15(1)
C(19)	10335(1)	3291(1)	6677(1)	19(1)
C(20)	10415(1)	3884(1)	5997(1)	23(1)
C(21)	10929(1)	4818(1)	6008(1)	26(1)
C(22)	11355(1)	5168(1)	6710(1)	24(1)
C(23)	11277(1)	4590(1)	7398(1)	20(1)

Table 3. Selected bond lengths [Å] and angles [°] for IAT41 (CCDC 752439).

Ta(1)-N(4)	1.7940(11)	N(4)-Ta(1)-N(1)	100.29(5)
Ta(1)-N(1)	2.0092(10)	N(4)-Ta(1)-N(3)	102.26(5)
Ta(1)-N(3)	2.0173(11)	N(1)-Ta(1)-N(3)	123.03(5)
Ta(1)-Cl(1)	2.3606(3)	N(4)-Ta(1)-Cl(1)	99.13(4)
Ta(1)-N(2)	2.3767(11)	N(1)-Ta(1)-Cl(1)	115.29(3)
		N(3)-Ta(1)-Cl(1)	111.69(4)
		N(4)-Ta(1)-N(2)	174.57(4)
		N(1)-Ta(1)-N(2)	76.10(4)
		N(3)-Ta(1)-N(2)	76.79(4)
		Cl(1)-Ta(1)-N(2)	86.14(3)

Table 4. Bond lengths [Å] and angles [°] for IAT41 (CCDC 752439).

Ta(1)-N(4)	1.7940(11)	C(11)-H(11C)	0.96(2)
Ta(1)-N(1)	2.0092(10)	C(12)-C(13)	1.398(2)
Ta(1)-N(3)	2.0173(11)	C(12)-C(17)	1.404(2)
Ta(1)-Cl(1)	2.3606(3)	C(13)-C(14)	1.388(2)
Ta(1)-N(2)	2.3767(11)	C(13)-H(13)	0.94(2)
Si(1)-N(1)	1.7576(12)	C(14)-C(15)	1.389(3)
Si(1)-C(7)	1.8593(17)	C(14)-H(14)	0.97(2)
Si(1)-C(8)	1.8590(16)	C(15)-C(16)	1.386(3)
Si(1)-C(6)	1.8761(17)	C(15)-H(15)	0.93(2)
Si(2)-N(3)	1.7572(12)	C(16)-C(17)	1.388(2)
Si(2)-C(11)	1.8526(16)	C(16)-H(16)	0.95(2)
Si(2)-C(10)	1.860(2)	C(17)-H(17)	0.98(2)
Si(2)-C(9)	1.885(2)	C(18)-C(19)	1.3932(19)
N(1)-C(1)	1.4797(17)	C(18)-C(23)	1.3983(18)
N(2)-C(5)	1.4743(18)	C(19)-C(20)	1.390(2)
N(2)-C(3)	1.4770(19)	C(19)-H(19)	0.970(19)
N(2)-C(2)	1.4854(18)	C(20)-C(21)	1.385(2)
N(3)-C(4)	1.4902(19)	C(20)-H(20)	0.98(2)
N(4)-N(5)	1.3641(15)	C(21)-C(22)	1.384(2)
N(5)-C(12)	1.3976(17)	C(21)-H(21)	0.94(2)
N(5)-C(18)	1.4150(16)	C(22)-C(23)	1.390(2)
C(1)-C(2)	1.505(2)	C(22)-H(22)	0.943(18)
C(1)-H(1A)	1.01(3)	C(23)-H(23)	0.92(2)
C(1)-H(1B)	0.933(18)		
C(2)-H(2A)	0.962(19)	N(4)-Ta(1)-N(1)	100.29(5)
C(2)-H(2B)	0.924(19)	N(4)-Ta(1)-N(3)	102.26(5)
C(3)-C(4)	1.511(2)	N(1)-Ta(1)-N(3)	123.03(5)
C(3)-H(3A)	1.023(19)	N(4)-Ta(1)-Cl(1)	99.13(4)
C(3)-H(3B)	0.96(2)	N(1)-Ta(1)-Cl(1)	115.29(3)
C(4)-H(4A)	1.007(19)	N(3)-Ta(1)-Cl(1)	111.69(4)
C(4)-H(4B)	1.01(3)	N(4)-Ta(1)-N(2)	174.57(4)
C(5)-H(5A)	0.99(2)	N(1)-Ta(1)-N(2)	76.10(4)
C(5)-H(5B)	0.981(18)	N(3)-Ta(1)-N(2)	76.79(4)
C(5)-H(5C)	0.95(2)	Cl(1)-Ta(1)-N(2)	86.14(3)
C(6)-H(6A)	1.00(3)	N(1)-Si(1)-C(7)	110.21(7)
C(6)-H(6B)	0.87(2)	N(1)-Si(1)-C(8)	112.80(6)
C(6)-H(6C)	0.95(3)	C(7)-Si(1)-C(8)	111.44(8)
C(7)-H(7A)	0.86(3)	N(1)-Si(1)-C(6)	108.11(7)
C(7)-H(7B)	0.98(2)	C(7)-Si(1)-C(6)	107.56(9)
C(7)-H(7C)	0.99(2)	C(8)-Si(1)-C(6)	106.46(9)
C(8)-H(8A)	0.97(2)	N(3)-Si(2)-C(11)	114.14(7)
C(8)-H(8B)	0.98(2)	N(3)-Si(2)-C(10)	110.90(8)
C(8)-H(8C)	0.90(2)	C(11)-Si(2)-C(10)	108.01(9)
C(9)-H(9A)	1.09(3)	N(3)-Si(2)-C(9)	106.72(8)
C(9)-H(9B)	1.02(4)	C(11)-Si(2)-C(9)	108.58(9)
C(9)-H(9C)	1.01(3)	C(10)-Si(2)-C(9)	108.32(11)
C(10)-H(10A)	1.10(3)	C(1)-N(1)-Si(1)	111.15(8)
C(10)-H(10B)	1.14(3)	C(1)-N(1)-Ta(1)	119.84(9)
C(10)-H(10C)	1.11(2)	Si(1)-N(1)-Ta(1)	128.98(6)
C(11)-H(11A)	0.94(2)	C(5)-N(2)-C(3)	110.19(12)
C(11)-H(11B)	0.94(2)	C(5)-N(2)-C(2)	109.54(11)

C(3)-N(2)-C(2)	110.44(12)	Si(1)-C(8)-H(8B)	108.6(11)
C(5)-N(2)-Ta(1)	118.30(9)	H(8A)-C(8)-H(8B)	108.4(17)
C(3)-N(2)-Ta(1)	106.22(8)	Si(1)-C(8)-H(8C)	113.2(13)
C(2)-N(2)-Ta(1)	101.76(8)	H(8A)-C(8)-H(8C)	105.1(18)
C(4)-N(3)-Si(2)	108.14(9)	H(8B)-C(8)-H(8C)	109.9(18)
C(4)-N(3)-Ta(1)	119.39(9)	Si(2)-C(9)-H(9A)	105.0(14)
Si(2)-N(3)-Ta(1)	131.11(6)	Si(2)-C(9)-H(9B)	110(2)
N(5)-N(4)-Ta(1)	177.51(9)	H(9A)-C(9)-H(9B)	112(2)
N(4)-N(5)-C(12)	118.96(10)	Si(2)-C(9)-H(9C)	106.6(17)
N(4)-N(5)-C(18)	117.04(11)	H(9A)-C(9)-H(9C)	113(2)
C(12)-N(5)-C(18)	123.99(11)	H(9B)-C(9)-H(9C)	110(3)
N(1)-C(1)-C(2)	110.53(11)	Si(2)-C(10)-H(10A)	112.6(16)
N(1)-C(1)-H(1A)	113.8(14)	Si(2)-C(10)-H(10B)	106.6(17)
C(2)-C(1)-H(1A)	104.2(14)	H(10A)-C(10)-H(10B)	111(2)
N(1)-C(1)-H(1B)	104.9(10)	Si(2)-C(10)-H(10C)	105.0(10)
C(2)-C(1)-H(1B)	108.4(11)	H(10A)-C(10)-H(10C)	104.9(18)
H(1A)-C(1)-H(1B)	115.1(17)	H(10B)-C(10)-H(10C)	116(2)
N(2)-C(2)-C(1)	108.54(12)	Si(2)-C(11)-H(11A)	113.7(11)
N(2)-C(2)-H(2A)	110.8(12)	Si(2)-C(11)-H(11B)	108.8(13)
C(1)-C(2)-H(2A)	113.2(11)	H(11A)-C(11)-H(11B)	103.9(18)
N(2)-C(2)-H(2B)	106.9(11)	Si(2)-C(11)-H(11C)	113.0(12)
C(1)-C(2)-H(2B)	111.2(11)	H(11A)-C(11)-H(11C)	105.6(16)
H(2A)-C(2)-H(2B)	106.0(15)	H(11B)-C(11)-H(11C)	111.4(17)
N(2)-C(3)-C(4)	109.13(12)	N(5)-C(12)-C(13)	120.56(13)
N(2)-C(3)-H(3A)	112.9(10)	N(5)-C(12)-C(17)	120.49(12)
C(4)-C(3)-H(3A)	108.6(11)	C(13)-C(12)-C(17)	118.92(13)
N(2)-C(3)-H(3B)	102.6(11)	C(14)-C(13)-C(12)	120.04(15)
C(4)-C(3)-H(3B)	112.7(11)	C(14)-C(13)-H(13)	122.9(13)
H(3A)-C(3)-H(3B)	110.9(16)	C(12)-C(13)-H(13)	117.0(13)
N(3)-C(4)-C(3)	110.03(13)	C(15)-C(14)-C(13)	120.96(15)
N(3)-C(4)-H(4A)	111.6(10)	C(15)-C(14)-H(14)	118.9(12)
C(3)-C(4)-H(4A)	106.1(12)	C(13)-C(14)-H(14)	120.1(12)
N(3)-C(4)-H(4B)	106.4(14)	C(14)-C(15)-C(16)	119.08(15)
C(3)-C(4)-H(4B)	112.8(13)	C(14)-C(15)-H(15)	120.4(12)
H(4A)-C(4)-H(4B)	110.0(18)	C(16)-C(15)-H(15)	120.5(12)
N(2)-C(5)-H(5A)	110.4(12)	C(17)-C(16)-C(15)	120.88(16)
N(2)-C(5)-H(5B)	111.2(11)	C(17)-C(16)-H(16)	116.7(13)
H(5A)-C(5)-H(5B)	106.9(14)	C(15)-C(16)-H(16)	122.4(13)
N(2)-C(5)-H(5C)	108.1(12)	C(16)-C(17)-C(12)	120.08(14)
H(5A)-C(5)-H(5C)	113.7(17)	C(16)-C(17)-H(17)	119.1(12)
H(5B)-C(5)-H(5C)	106.5(16)	C(12)-C(17)-H(17)	120.6(12)
Si(1)-C(6)-H(6A)	109.6(13)	C(19)-C(18)-C(23)	119.58(12)
Si(1)-C(6)-H(6B)	107.0(14)	C(19)-C(18)-N(5)	119.82(11)
H(6A)-C(6)-H(6B)	111(2)	C(23)-C(18)-N(5)	120.56(12)
Si(1)-C(6)-H(6C)	107.2(14)	C(20)-C(19)-C(18)	119.78(13)
H(6A)-C(6)-H(6C)	115(2)	C(20)-C(19)-H(19)	120.7(12)
H(6B)-C(6)-H(6C)	107(2)	C(18)-C(19)-H(19)	119.4(12)
Si(1)-C(7)-H(7A)	112.2(17)	C(21)-C(20)-C(19)	120.82(15)
Si(1)-C(7)-H(7B)	110.0(15)	C(21)-C(20)-H(20)	121.4(11)
H(7A)-C(7)-H(7B)	118(2)	C(19)-C(20)-H(20)	117.8(11)
Si(1)-C(7)-H(7C)	108.8(14)	C(22)-C(21)-C(20)	119.32(13)
H(7A)-C(7)-H(7C)	103(2)	C(22)-C(21)-H(21)	120.0(12)
H(7B)-C(7)-H(7C)	104.9(19)	C(20)-C(21)-H(21)	120.6(12)
Si(1)-C(8)-H(8A)	111.4(13)	C(21)-C(22)-C(23)	120.78(14)

C(21)-C(22)-H(22)	121.8(11)	C(22)-C(23)-H(23)	122.7(11)
C(23)-C(22)-H(22)	117.3(11)	C(18)-C(23)-H(23)	117.6(11)
C(22)-C(23)-C(18)	119.70(14)		

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for IAT41 (CCDC 752439). The anisotropic displacement factorexponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	131(1)	117(1)	123(1)	3(1)	-2(1)	-16(1)
Cl(1)	228(2)	254(1)	173(1)	53(1)	-48(1)	1(1)
Si(1)	153(2)	164(2)	217(2)	-6(1)	-6(1)	14(1)
Si(2)	297(2)	214(2)	245(2)	-77(2)	64(2)	-64(2)
N(1)	149(5)	136(4)	215(5)	16(4)	3(4)	-15(3)
N(2)	136(5)	180(4)	182(5)	-8(4)	-12(4)	-24(4)
N(3)	199(5)	174(5)	188(5)	-22(4)	51(4)	-42(4)
N(4)	163(5)	156(4)	137(5)	0(3)	10(4)	-36(3)
N(5)	162(5)	193(4)	133(4)	37(4)	-11(4)	-72(4)
C(1)	198(6)	153(5)	344(8)	30(5)	23(6)	-24(4)
C(2)	200(6)	200(6)	229(7)	42(5)	9(5)	-49(5)
C(3)	172(6)	236(6)	281(7)	-7(5)	33(5)	-8(5)
C(4)	239(7)	238(6)	263(7)	-59(6)	94(6)	-57(5)
C(5)	220(7)	315(7)	225(7)	-38(6)	-26(5)	-92(6)
C(6)	270(8)	222(7)	459(11)	-80(7)	43(8)	22(6)
C(7)	215(7)	330(8)	278(8)	15(6)	-38(6)	27(6)
C(8)	244(7)	254(7)	265(7)	11(6)	63(6)	37(6)
C(9)	331(10)	281(8)	557(13)	1(8)	68(9)	4(7)
C(10)	576(13)	454(11)	251(8)	-119(8)	74(9)	-163(10)
C(11)	288(8)	179(6)	260(7)	-24(5)	23(6)	-52(5)
C(12)	189(6)	138(5)	157(5)	8(4)	-33(4)	-28(4)
C(13)	269(7)	197(6)	170(6)	32(5)	-32(5)	-76(5)
C(14)	384(9)	207(6)	189(7)	45(5)	-89(6)	-61(6)
C(15)	335(8)	240(6)	283(8)	19(6)	-159(7)	16(6)
C(16)	202(7)	292(7)	313(8)	-17(6)	-73(6)	27(5)
C(17)	179(6)	230(6)	207(6)	-1(5)	-27(5)	5(5)
C(18)	136(5)	182(5)	145(5)	31(4)	22(4)	-4(4)
C(19)	186(6)	227(6)	148(5)	11(4)	14(5)	11(4)
C(20)	204(6)	335(7)	145(6)	33(5)	25(5)	70(5)
C(21)	203(7)	338(7)	234(7)	143(6)	79(5)	82(6)
C(22)	181(6)	222(6)	324(8)	111(6)	59(6)	5(5)
C(23)	172(6)	196(5)	230(7)	40(5)	11(5)	-23(4)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for IAT41 (CCDC 752439).

	x	y	z	U_{iso}
H(1A)	8650(20)	-784(18)	9163(16)	55(7)
H(1B)	8153(13)	-740(12)	8272(10)	14(4)
H(2A)	6884(15)	-353(14)	9172(11)	24(5)
H(2B)	7571(14)	455(13)	9534(11)	20(4)
H(3A)	5776(15)	1287(14)	9202(11)	25(5)
H(3B)	6087(15)	2073(13)	8488(12)	22(5)
H(4A)	6485(15)	2858(14)	9686(12)	23(5)
H(4B)	7180(20)	1867(15)	9983(16)	45(7)
H(5A)	5979(16)	-2(14)	8012(12)	29(5)
H(5B)	7000(14)	39(13)	7523(11)	19(4)
H(5C)	6296(15)	994(14)	7490(12)	28(5)
H(6A)	9750(20)	-1883(16)	8278(16)	48(7)
H(6B)	10635(19)	-1698(16)	7704(14)	37(6)
H(6C)	9638(19)	-1423(17)	7380(15)	45(6)
H(7A)	11164(19)	433(19)	9304(15)	48(7)
H(7B)	11668(19)	-593(18)	9002(14)	49(6)
H(7C)	10687(18)	-533(17)	9517(14)	41(6)
H(8A)	10448(17)	717(16)	6939(13)	39(6)
H(8B)	11478(16)	160(14)	7199(12)	28(5)
H(8C)	11142(16)	1215(16)	7526(13)	32(5)
H(9A)	6800(20)	4470(20)	8469(17)	65(8)
H(9B)	7030(30)	5490(30)	9130(20)	99(11)
H(9C)	6310(20)	4520(20)	9430(18)	76(9)
H(10A)	7430(20)	3710(20)	10823(17)	73(8)
H(10B)	8130(30)	4930(20)	10699(19)	90(10)
H(10C)	8751(16)	3597(14)	10732(12)	26(5)
H(11A)	9821(16)	4359(14)	9287(11)	25(5)
H(11B)	9212(17)	5319(17)	9226(13)	41(6)
H(11C)	9280(15)	4552(14)	8512(12)	27(5)
H(13)	10497(16)	2651(15)	9549(12)	31(5)
H(14)	11790(15)	2484(15)	10544(13)	31(5)
H(15)	13491(15)	2683(14)	10188(12)	28(5)
H(16)	13912(17)	3030(13)	8859(12)	26(5)
H(17)	12671(15)	3154(12)	7903(13)	23(5)
H(19)	9948(15)	2653(14)	6674(11)	25(5)
H(20)	10090(15)	3620(14)	5511(12)	25(5)
H(21)	10964(15)	5225(14)	5553(12)	30(5)
H(22)	11685(14)	5813(14)	6746(11)	21(4)
H(23)	11531(14)	4815(13)	7876(11)	21(4)

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 3 February 2009

Crystal Structure Analysis of:

Complex 11 (IAT29)

(shown below)

For Investigator: Ian Tonks ext. 6576

Advisor: J. E. Bercaw ext. 6577

By Michael W. Day 116 Beckman ext. 2734

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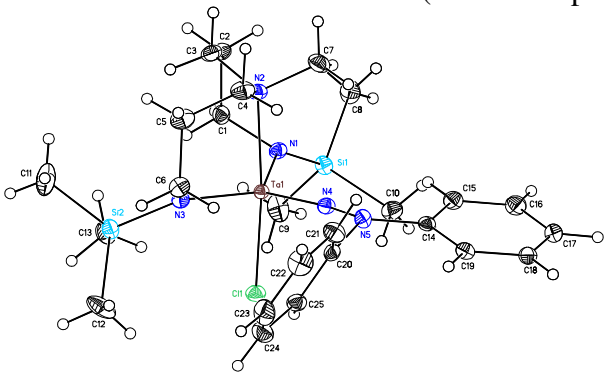
Contents



IAT29

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC). The deposition number is 719036.

Table 1. Crystal data and structure refinement for IAT29 (CCDC 719036).

Empirical formula	$C_{25}H_{43}N_5Si_2ClTa$
Formula weight	686.22
Crystallization Solvent	Dichloromethane/pentane
Crystal Habit	Blade
Crystal size	0.29 x 0.14 x 0.06 mm^3
Crystal color	Yellow/orange

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 9461 reflections used in lattice determination	2.28 to 38.42°
Unit cell dimensions	a = 8.1959(4) Å b = 10.4496(5) Å β= 94.059(2)° c = 34.5115(14) Å
Volume	2948.3(2) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.546 Mg/m^3
F(000)	1384
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	2.04 to 38.82°
Completeness to θ = 38.82°	73.0 %
Index ranges	$-14 \le h \le 9$, $-16 \le k \le 16$, $-52 \le l \le 53$
Data collection scan type	ω scans; 22 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	82761
Independent reflections	12381 [R_{int}= 0.0302]
Absorption coefficient	3.922 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7476 and 0.5387

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	12381 / 0 / 479
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.754
Final R indices [$I>2\sigma(I)$, 10825 reflections]	R1 = 0.0235, *w*R2 = 0.0341
R indices (all data)	R1 = 0.0309, *w*R2 = 0.0345
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	1.963 and -1.707 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

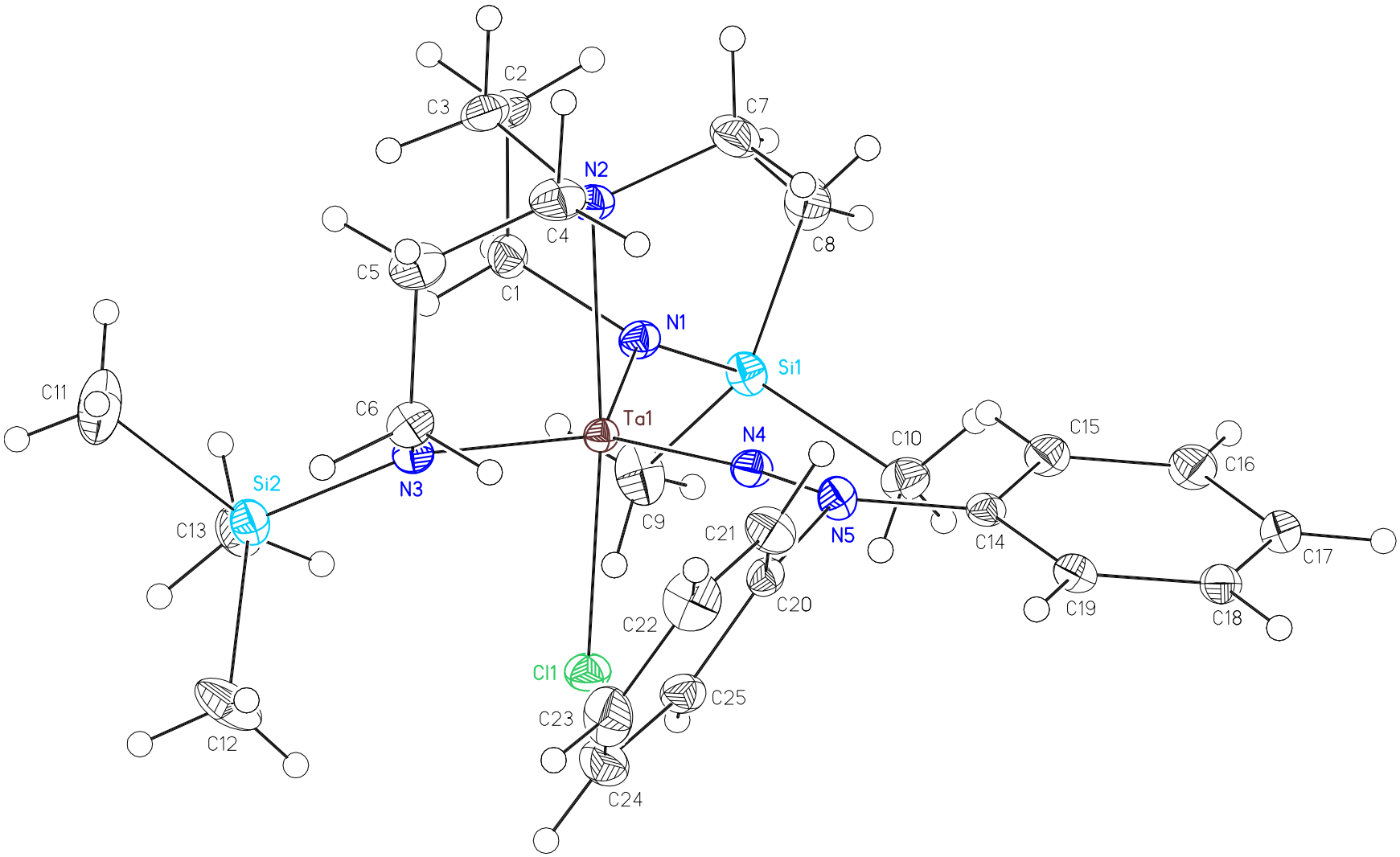

C2
C3
C7
N2
C4
C8
C5
C1
N1
Si1
C11
C6
Ta1
N4
C10
C15
C16
Si2
N3
C9
C13
C21
N5
C14
C17
C20
C19
C18
C22
Cl1
C25
C23
C12
C24

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT29 (CCDC 719036). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	5000(1)	1565(1)	1404(1)	11(1)
Cl(1)	7467(1)	2512(1)	1721(1)	17(1)
Si(1)	5781(1)	-511(1)	2181(1)	15(1)
Si(2)	3868(1)	4662(1)	1548(1)	17(1)
N(1)	4593(1)	447(1)	1860(1)	14(1)
N(2)	2489(1)	762(1)	1157(1)	15(1)
N(3)	3982(1)	3268(1)	1270(1)	14(1)
N(4)	5954(1)	834(1)	1009(1)	14(1)
N(5)	6515(1)	575(1)	652(1)	15(1)
C(1)	3098(2)	985(2)	2024(1)	16(1)
C(2)	1514(2)	463(2)	1832(1)	20(1)
C(3)	1142(2)	987(2)	1425(1)	19(1)
C(4)	1987(2)	1339(2)	769(1)	21(1)
C(5)	1802(2)	2781(2)	753(1)	22(1)
C(6)	3394(2)	3487(2)	857(1)	18(1)
C(7)	2635(2)	-636(2)	1092(1)	22(1)
C(8)	4560(2)	-1910(2)	2331(1)	26(1)
C(9)	6428(2)	451(2)	2619(1)	26(1)
C(10)	7601(2)	-1102(2)	1944(1)	20(1)
C(11)	1788(2)	5394(2)	1471(1)	38(1)
C(12)	5421(3)	5810(2)	1383(1)	32(1)
C(13)	4244(2)	4361(2)	2076(1)	22(1)
C(14)	7483(1)	-528(1)	610(1)	13(1)
C(15)	7498(2)	-1493(1)	888(1)	18(1)
C(16)	8454(2)	-2576(2)	853(1)	20(1)
C(17)	9404(2)	-2726(2)	539(1)	19(1)
C(18)	9374(2)	-1779(1)	260(1)	17(1)
C(19)	8423(2)	-688(2)	289(1)	15(1)
C(20)	6705(2)	1702(1)	418(1)	14(1)
C(21)	6022(2)	1754(2)	38(1)	21(1)
C(22)	6106(2)	2878(2)	-172(1)	27(1)
C(23)	6861(2)	3950(2)	-5(1)	27(1)
C(24)	7549(2)	3891(2)	372(1)	24(1)
C(25)	7478(2)	2769(2)	584(1)	17(1)

Table 3. Selected bond lengths [Å] and angles [°] for IAT29 (CCDC 719036).

Ta(1)-N(4)	1.7909(11)	N(4)-Ta(1)-N(3)	113.52(5)
Ta(1)-N(3)	2.0056(11)	N(4)-Ta(1)-N(1)	116.99(5)
Ta(1)-N(1)	2.0044(11)	N(3)-Ta(1)-N(1)	127.53(4)
Ta(1)-N(2)	2.3276(11)	N(4)-Ta(1)-N(2)	89.41(4)
Ta(1)-Cl(1)	2.4390(3)	N(3)-Ta(1)-N(2)	83.84(4)
		N(1)-Ta(1)-N(2)	83.41(4)
		N(4)-Ta(1)-Cl(1)	96.96(4)
		N(3)-Ta(1)-Cl(1)	93.55(3)
		N(1)-Ta(1)-Cl(1)	93.66(3)
		N(2)-Ta(1)-Cl(1)	173.62(3)

Table 4. Bond lengths [Å] and angles [°] for IAT29 (CCDC 719036).

Ta(1)-N(4)	1.7909(11)	C(11)-H(11C)	0.95(2)
Ta(1)-N(3)	2.0056(11)	C(12)-H(12A)	0.943(19)
Ta(1)-N(1)	2.0044(11)	C(12)-H(12B)	0.92(2)
Ta(1)-N(2)	2.3276(11)	C(12)-H(12C)	0.94(2)
Ta(1)-Cl(1)	2.4390(3)	C(13)-H(13A)	0.900(18)
Si(1)-N(1)	1.7405(12)	C(13)-H(13B)	0.99(2)
Si(1)-C(10)	1.8577(15)	C(13)-H(13C)	0.929(19)
Si(1)-C(9)	1.8612(17)	C(14)-C(15)	1.3917(19)
Si(1)-C(8)	1.8658(17)	C(14)-C(19)	1.4022(18)
Si(2)-N(3)	1.7503(12)	C(15)-C(16)	1.386(2)
Si(2)-C(13)	1.8546(17)	C(15)-H(15)	0.930(15)
Si(2)-C(12)	1.8672(17)	C(16)-C(17)	1.390(2)
Si(2)-C(11)	1.8702(18)	C(16)-H(16)	0.937(16)
N(1)-C(1)	1.4962(16)	C(17)-C(18)	1.380(2)
N(2)-C(7)	1.485(2)	C(17)-H(17)	0.977(15)
N(2)-C(4)	1.5016(19)	C(18)-C(19)	1.389(2)
N(2)-C(3)	1.5074(17)	C(18)-H(18)	0.967(14)
N(3)-C(6)	1.4876(18)	C(19)-H(19)	0.904(14)
N(4)-N(5)	1.3743(15)	C(20)-C(21)	1.389(2)
N(5)-C(14)	1.4124(17)	C(20)-C(25)	1.385(2)
N(5)-C(20)	1.4422(18)	C(21)-C(22)	1.386(2)
C(1)-C(2)	1.517(2)	C(21)-H(21)	0.896(17)
C(1)-H(1A)	0.944(15)	C(22)-C(23)	1.386(3)
C(1)-H(1B)	0.987(16)	C(22)-H(22)	0.935(18)
C(2)-C(3)	1.517(2)	C(23)-C(24)	1.380(2)
C(2)-H(2A)	0.970(14)	C(23)-H(23)	0.905(17)
C(2)-H(2B)	0.945(15)	C(24)-C(25)	1.385(2)
C(3)-H(3A)	0.978(15)	C(24)-H(24)	0.936(17)
C(3)-H(3B)	0.990(16)	C(25)-H(25)	0.967(16)
C(4)-C(5)	1.514(2)		
C(4)-H(4A)	0.961(16)	N(4)-Ta(1)-N(3)	113.52(5)
C(4)-H(4B)	0.961(14)	N(4)-Ta(1)-N(1)	116.99(5)
C(5)-C(6)	1.520(2)	N(3)-Ta(1)-N(1)	127.53(4)
C(5)-H(5A)	0.926(18)	N(4)-Ta(1)-N(2)	89.41(4)
C(5)-H(5B)	1.005(14)	N(3)-Ta(1)-N(2)	83.84(4)
C(6)-H(6A)	0.993(14)	N(1)-Ta(1)-N(2)	83.41(4)
C(6)-H(6B)	1.020(16)	N(4)-Ta(1)-Cl(1)	96.96(4)
C(7)-H(7A)	0.951(16)	N(3)-Ta(1)-Cl(1)	93.55(3)
C(7)-H(7B)	0.944(17)	N(1)-Ta(1)-Cl(1)	93.66(3)
C(7)-H(7C)	0.949(15)	N(2)-Ta(1)-Cl(1)	173.62(3)
C(8)-H(8A)	0.86(2)	N(1)-Si(1)-C(10)	109.90(7)
C(8)-H(8B)	0.88(2)	N(1)-Si(1)-C(9)	108.76(7)
C(8)-H(8C)	0.98(2)	C(10)-Si(1)-C(9)	110.30(8)
C(9)-H(9A)	0.954(19)	N(1)-Si(1)-C(8)	109.93(8)
C(9)-H(9B)	0.93(2)	C(10)-Si(1)-C(8)	108.94(8)
C(9)-H(9C)	0.919(18)	C(9)-Si(1)-C(8)	109.00(9)
C(10)-H(10A)	0.930(19)	N(3)-Si(2)-C(13)	112.75(7)
C(10)-H(10B)	0.91(2)	N(3)-Si(2)-C(12)	107.67(8)
C(10)-H(10C)	0.956(19)	C(13)-Si(2)-C(12)	109.81(9)
C(11)-H(11A)	0.94(2)	N(3)-Si(2)-C(11)	110.25(9)
C(11)-H(11B)	0.89(2)	C(13)-Si(2)-C(11)	107.15(9)

C(12)-Si(2)-C(11)	109.18(11)	N(2)-C(7)-H(7B)	110.6(10)
C(1)-N(1)-Si(1)	114.19(9)	H(7A)-C(7)-H(7B)	107.6(13)
C(1)-N(1)-Ta(1)	105.37(9)	N(2)-C(7)-H(7C)	110.4(10)
Si(1)-N(1)-Ta(1)	135.94(6)	H(7A)-C(7)-H(7C)	109.4(13)
C(7)-N(2)-C(4)	106.17(12)	H(7B)-C(7)-H(7C)	107.8(13)
C(7)-N(2)-C(3)	108.55(12)	Si(1)-C(8)-H(8A)	114.3(14)
C(4)-N(2)-C(3)	108.60(11)	Si(1)-C(8)-H(8B)	111.4(12)
C(7)-N(2)-Ta(1)	109.40(9)	H(8A)-C(8)-H(8B)	109.6(19)
C(4)-N(2)-Ta(1)	111.20(8)	Si(1)-C(8)-H(8C)	111.9(11)
C(3)-N(2)-Ta(1)	112.69(9)	H(8A)-C(8)-H(8C)	103.2(18)
C(6)-N(3)-Si(2)	111.77(9)	H(8B)-C(8)-H(8C)	105.9(17)
C(6)-N(3)-Ta(1)	117.33(9)	Si(1)-C(9)-H(9A)	110.4(12)
Si(2)-N(3)-Ta(1)	130.43(6)	Si(1)-C(9)-H(9B)	110.3(12)
N(5)-N(4)-Ta(1)	163.75(10)	H(9A)-C(9)-H(9B)	108.1(15)
N(4)-N(5)-C(14)	118.59(11)	Si(1)-C(9)-H(9C)	111.8(12)
N(4)-N(5)-C(20)	113.41(11)	H(9A)-C(9)-H(9C)	108.5(16)
C(14)-N(5)-C(20)	121.72(10)	H(9B)-C(9)-H(9C)	107.5(15)
N(1)-C(1)-C(2)	113.40(12)	Si(1)-C(10)-H(10A)	111.2(10)
N(1)-C(1)-H(1A)	110.2(8)	Si(1)-C(10)-H(10B)	109.0(11)
C(2)-C(1)-H(1A)	106.1(9)	H(10A)-C(10)-H(10B)	107.4(15)
N(1)-C(1)-H(1B)	111.1(9)	Si(1)-C(10)-H(10C)	111.3(10)
C(2)-C(1)-H(1B)	109.3(9)	H(10A)-C(10)-H(10C)	108.2(15)
H(1A)-C(1)-H(1B)	106.4(13)	H(10B)-C(10)-H(10C)	109.7(15)
C(1)-C(2)-C(3)	112.65(12)	Si(2)-C(11)-H(11A)	110.3(12)
C(1)-C(2)-H(2A)	109.2(9)	Si(2)-C(11)-H(11B)	110.1(14)
C(3)-C(2)-H(2A)	106.7(9)	H(11A)-C(11)-H(11B)	110(2)
C(1)-C(2)-H(2B)	110.5(9)	Si(2)-C(11)-H(11C)	113.0(12)
C(3)-C(2)-H(2B)	111.1(9)	H(11A)-C(11)-H(11C)	108.1(18)
H(2A)-C(2)-H(2B)	106.4(12)	H(11B)-C(11)-H(11C)	104.8(17)
N(2)-C(3)-C(2)	113.76(12)	Si(2)-C(12)-H(12A)	108.8(12)
N(2)-C(3)-H(3A)	106.5(8)	Si(2)-C(12)-H(12B)	113.7(12)
C(2)-C(3)-H(3A)	112.6(9)	H(12A)-C(12)-H(12B)	106.4(18)
N(2)-C(3)-H(3B)	107.6(8)	Si(2)-C(12)-H(12C)	108.9(14)
C(2)-C(3)-H(3B)	109.9(9)	H(12A)-C(12)-H(12C)	108.4(16)
H(3A)-C(3)-H(3B)	106.0(13)	H(12B)-C(12)-H(12C)	110.6(19)
N(2)-C(4)-C(5)	116.85(13)	Si(2)-C(13)-H(13A)	110.8(12)
N(2)-C(4)-H(4A)	107.6(10)	Si(2)-C(13)-H(13B)	107.5(11)
C(5)-C(4)-H(4A)	111.2(10)	H(13A)-C(13)-H(13B)	109.0(15)
N(2)-C(4)-H(4B)	105.5(9)	Si(2)-C(13)-H(13C)	114.4(11)
C(5)-C(4)-H(4B)	111.3(9)	H(13A)-C(13)-H(13C)	107.0(16)
H(4A)-C(4)-H(4B)	103.4(13)	H(13B)-C(13)-H(13C)	108.1(15)
C(6)-C(5)-C(4)	113.08(13)	C(15)-C(14)-C(19)	118.67(13)
C(6)-C(5)-H(5A)	109.0(10)	C(15)-C(14)-N(5)	119.89(12)
C(4)-C(5)-H(5A)	107.4(11)	C(19)-C(14)-N(5)	121.43(13)
C(6)-C(5)-H(5B)	108.4(9)	C(16)-C(15)-C(14)	120.60(13)
C(4)-C(5)-H(5B)	110.7(9)	C(16)-C(15)-H(15)	120.5(10)
H(5A)-C(5)-H(5B)	108.1(13)	C(14)-C(15)-H(15)	118.9(10)
N(3)-C(6)-C(5)	111.52(12)	C(17)-C(16)-C(15)	120.73(15)
N(3)-C(6)-H(6A)	112.2(9)	C(17)-C(16)-H(16)	121.4(9)
C(5)-C(6)-H(6A)	108.6(9)	C(15)-C(16)-H(16)	117.9(9)
N(3)-C(6)-H(6B)	111.7(9)	C(18)-C(17)-C(16)	118.78(14)
C(5)-C(6)-H(6B)	110.0(8)	C(18)-C(17)-H(17)	120.4(9)
H(6A)-C(6)-H(6B)	102.4(11)	C(16)-C(17)-H(17)	120.9(9)
N(2)-C(7)-H(7A)	110.9(10)	C(17)-C(18)-C(19)	121.32(13)

C(17)-C(18)-H(18)	120.9(9)	C(21)-C(22)-H(22)	120.0(12)
C(19)-C(18)-H(18)	117.8(9)	C(23)-C(22)-H(22)	119.8(12)
C(18)-C(19)-C(14)	119.89(14)	C(24)-C(23)-C(22)	119.87(16)
C(18)-C(19)-H(19)	120.7(8)	C(24)-C(23)-H(23)	119.7(11)
C(14)-C(19)-H(19)	119.4(9)	C(22)-C(23)-H(23)	120.4(11)
C(21)-C(20)-C(25)	119.95(14)	C(23)-C(24)-C(25)	120.29(16)
C(21)-C(20)-N(5)	120.47(13)	C(23)-C(24)-H(24)	118.6(10)
C(25)-C(20)-N(5)	119.42(13)	C(25)-C(24)-H(24)	121.1(10)
C(22)-C(21)-C(20)	119.78(15)	C(20)-C(25)-C(24)	119.92(15)
C(22)-C(21)-H(21)	118.5(11)	C(20)-C(25)-H(25)	118.1(9)
C(20)-C(21)-H(21)	121.7(11)	C(24)-C(25)-H(25)	121.8(10)
C(21)-C(22)-C(23)	120.18(16)		

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT29 (CCDC 719036). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	105(1)	118(1)	94(1)	-4(1)	16(1)	-4(1)
Cl(1)	137(1)	191(2)	175(2)	-16(1)	-17(1)	-23(1)
Si(1)	192(2)	135(2)	128(2)	16(2)	26(1)	-2(2)
Si(2)	204(2)	134(2)	172(2)	-1(2)	33(2)	9(2)
N(1)	133(5)	162(6)	130(5)	-2(5)	28(4)	-10(4)
N(2)	133(5)	186(7)	144(6)	-26(5)	14(4)	-31(4)
N(3)	130(5)	149(6)	125(5)	8(5)	-3(4)	-3(4)
N(4)	145(5)	169(6)	122(5)	-30(5)	39(4)	-28(4)
N(5)	190(5)	145(6)	109(5)	-4(5)	58(4)	-3(4)
C(1)	183(6)	159(8)	157(7)	-17(6)	44(5)	3(5)
C(2)	157(6)	208(9)	232(8)	-12(7)	68(6)	-31(6)
C(3)	122(6)	244(9)	218(8)	-31(7)	24(5)	-27(6)
C(4)	178(6)	295(10)	155(7)	-31(7)	-38(6)	-49(6)
C(5)	184(7)	298(10)	168(7)	16(7)	-49(6)	-8(6)
C(6)	178(6)	213(8)	146(7)	24(7)	-11(5)	11(6)
C(7)	231(7)	200(9)	224(8)	-57(7)	9(6)	-62(6)
C(8)	291(8)	182(9)	321(10)	62(8)	142(8)	17(7)
C(9)	365(9)	230(9)	170(8)	-9(7)	-35(7)	50(8)
C(10)	167(6)	216(8)	205(8)	22(7)	2(6)	-5(6)
C(11)	373(10)	339(12)	434(13)	-65(11)	10(9)	185(9)
C(12)	466(11)	213(10)	276(10)	26(8)	76(8)	-166(8)
C(13)	299(8)	191(9)	190(8)	-24(7)	79(7)	-21(7)
C(14)	121(5)	146(7)	118(6)	-30(6)	4(5)	-27(5)
C(15)	188(6)	185(8)	157(7)	-3(6)	56(5)	-26(6)
C(16)	206(7)	180(8)	217(8)	53(7)	38(6)	-12(6)
C(17)	171(6)	165(8)	234(8)	-32(7)	22(6)	-2(6)
C(18)	163(6)	183(8)	162(7)	-57(6)	44(5)	-27(5)
C(19)	175(6)	153(7)	127(7)	-5(6)	18(5)	-31(5)
C(20)	135(5)	150(7)	143(6)	-2(6)	41(5)	5(5)
C(21)	243(7)	208(9)	164(7)	-11(7)	-7(6)	-30(6)
C(22)	320(8)	313(10)	176(8)	66(8)	-5(7)	32(7)
C(23)	336(8)	192(9)	290(9)	108(8)	95(7)	48(7)
C(24)	264(8)	181(8)	276(9)	-4(7)	71(7)	-45(6)
C(25)	158(6)	198(8)	169(7)	-13(6)	38(5)	-28(5)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for IAT29 (CCDC 719036).

	x	y	z	U_{iso}
H(1A)	3056(16)	1880(15)	1988(4)	11(4)
H(1B)	3119(17)	837(15)	2307(5)	22(4)
H(2A)	612(17)	714(15)	1982(4)	18(4)
H(2B)	1528(16)	-441(15)	1831(4)	11(4)
H(3A)	147(17)	621(15)	1297(4)	19(4)
H(3B)	953(17)	1922(16)	1437(5)	17(4)
H(4A)	999(19)	920(16)	671(5)	26(4)
H(4B)	2784(17)	1049(15)	598(4)	18(4)
H(5A)	1429(19)	2996(17)	502(5)	30(5)
H(5B)	966(17)	3076(15)	933(4)	18(4)
H(6A)	4211(17)	3219(14)	674(4)	12(4)
H(6B)	3254(17)	4437(16)	797(4)	18(4)
H(7A)	1603(19)	-999(16)	1010(5)	25(4)
H(7B)	3018(17)	-1054(16)	1323(5)	19(4)
H(7C)	3391(18)	-801(15)	901(5)	21(4)
H(8A)	3640(30)	-1710(20)	2424(7)	60(7)
H(8B)	5130(20)	-2400(20)	2497(6)	45(6)
H(8C)	4220(20)	-2465(19)	2109(6)	46(6)
H(9A)	7130(20)	1131(19)	2553(5)	42(6)
H(9B)	6990(20)	-59(19)	2803(6)	40(5)
H(9C)	5550(20)	795(18)	2733(5)	38(5)
H(10A)	7340(20)	-1801(18)	1785(5)	32(5)
H(10B)	8370(20)	-1366(17)	2130(6)	37(5)
H(10C)	8050(20)	-450(19)	1789(5)	40(5)
H(11A)	1570(20)	5610(20)	1209(7)	58(7)
H(11B)	1720(30)	6080(20)	1622(7)	60(7)
H(11C)	940(20)	4840(20)	1544(6)	49(6)
H(12A)	6470(20)	5491(19)	1457(6)	43(6)
H(12B)	5360(20)	6610(20)	1494(7)	58(7)
H(12C)	5310(30)	5870(20)	1110(7)	69(7)
H(13A)	3350(20)	4029(18)	2175(5)	39(5)
H(13B)	4500(20)	5200(20)	2204(5)	41(5)
H(13C)	5100(20)	3804(18)	2141(5)	35(5)
H(15)	6874(18)	-1391(14)	1101(5)	20(4)
H(16)	8472(18)	-3182(15)	1054(5)	19(4)
H(17)	10086(17)	-3485(14)	515(5)	17(4)
H(18)	10001(16)	-1862(14)	34(4)	13(4)
H(19)	8426(15)	-65(14)	108(4)	8(4)
H(21)	5496(19)	1084(17)	-73(5)	26(5)
H(22)	5650(20)	2915(18)	-429(5)	34(5)
H(23)	6880(17)	4695(16)	-138(5)	21(4)
H(24)	8044(18)	4627(16)	481(5)	24(4)
H(25)	7886(17)	2720(15)	853(5)	18(4)

CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 10 July 2009

Crystal Structure Analysis of:

Complex 13 (IAT37)

(shown below)

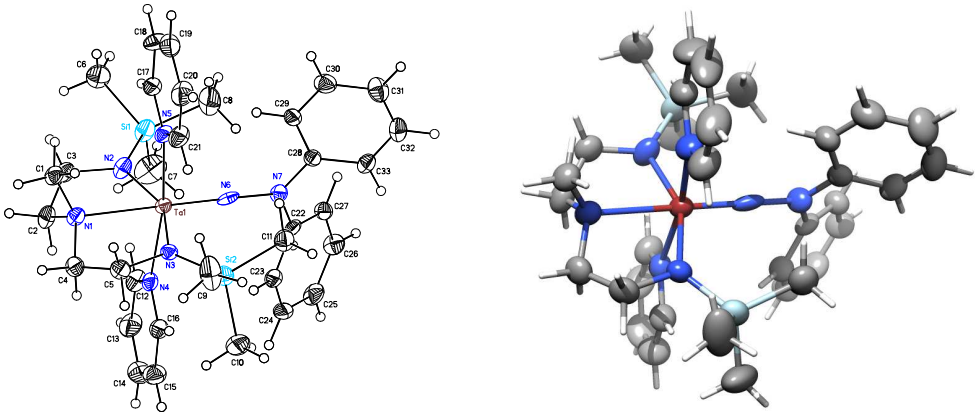
For Investigator: Ian Tonks ext. 6576

Advisor: J. E. Bercaw ext. 6577

By Michael W. Day 116 Beckman ext. 2734

e-mail: mikeday@caltech.edu

Contents



IAT37

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC). The deposition number is 739782.

Table 1. Crystal data and structure refinement for IAT37 (CCDC 739782).

Empirical formula	$[C_{33}H_{49}N_7Si_2Ta]^+ [C_{32}H_{12}BF_{24}]^-$
Formula weight	1644.15
Crystallization Solvent	Pentane/dichloromethane
Crystal Habit	Flake
Crystal size	0.48 x 0.38 x 0.01 mm^3
Crystal color	Orange

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9768 reflections used in lattice determination	2.18 to 27.14°
Unit cell dimensions	a = 22.0650(16) Å b = 13.9417(10) Å β= 114.312(4)° c = 24.4542(16) Å
Volume	6855.6(8) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.593 Mg/m^3
F(000)	3288
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	1.62 to 27.70°
Completeness to θ = 27.70°	89.8 %
Index ranges	$-28 \le h \le 25$, $-17 \le k \le 18$, $-31 \le l \le 31$
Data collection scan type	ω scans; 12 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	99951
Independent reflections	14430 [R_{int}= 0.0757]
Absorption coefficient	1.750 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.5719

Table 1 (cont.)

Structure solution and Refinement

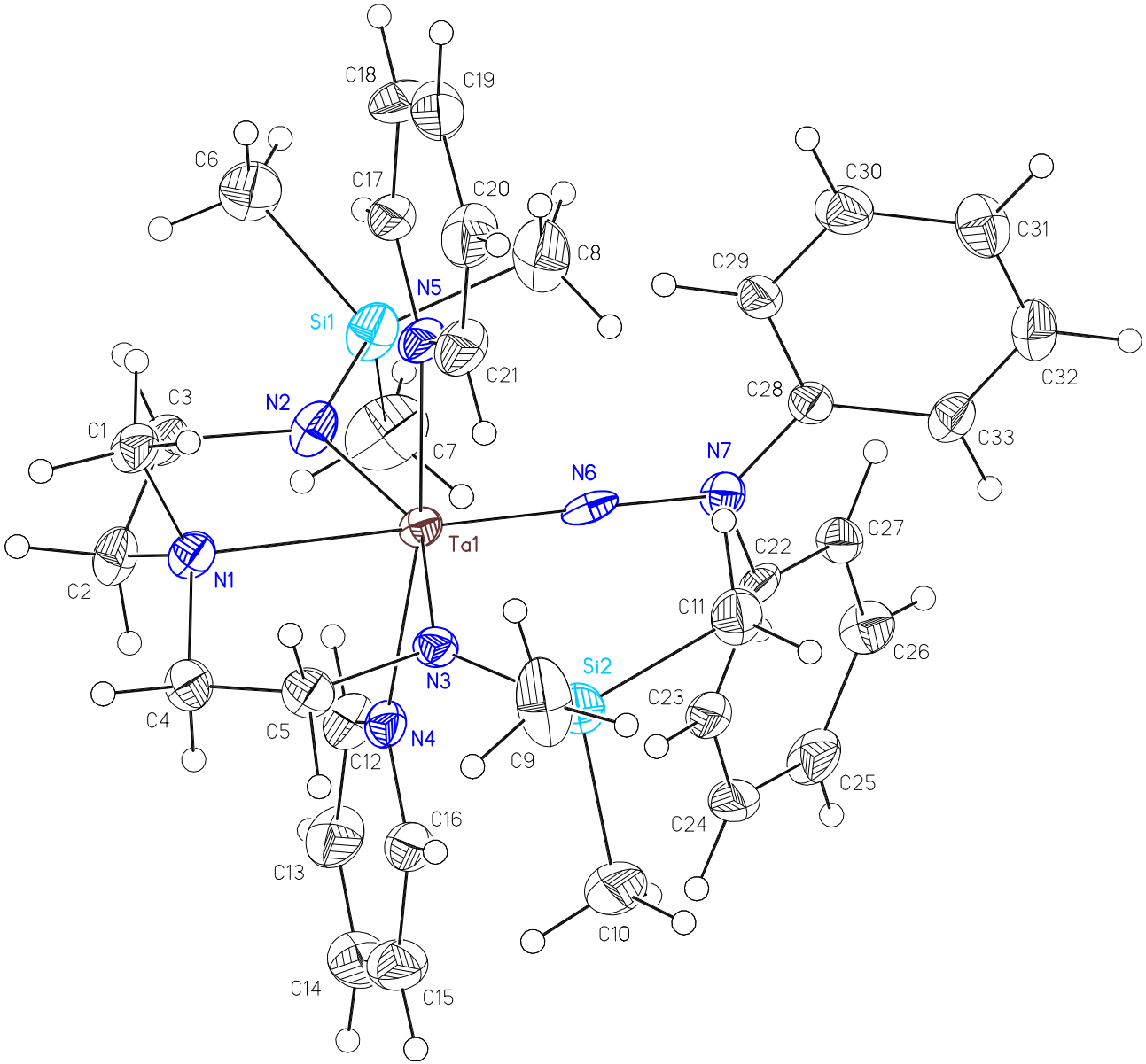
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	14430 / 0 / 908
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.652
Final R indices [$I>2\sigma(I)$, 10334 reflections]	R1 = 0.0387, *w*R2 = 0.0666
R indices (all data)	R1 = 0.0764, *w*R2 = 0.0718
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	1.530 and -1.207 e.Å^{-3}

Special Refinement Details

Crystals were mounted in a loop using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C11
C26
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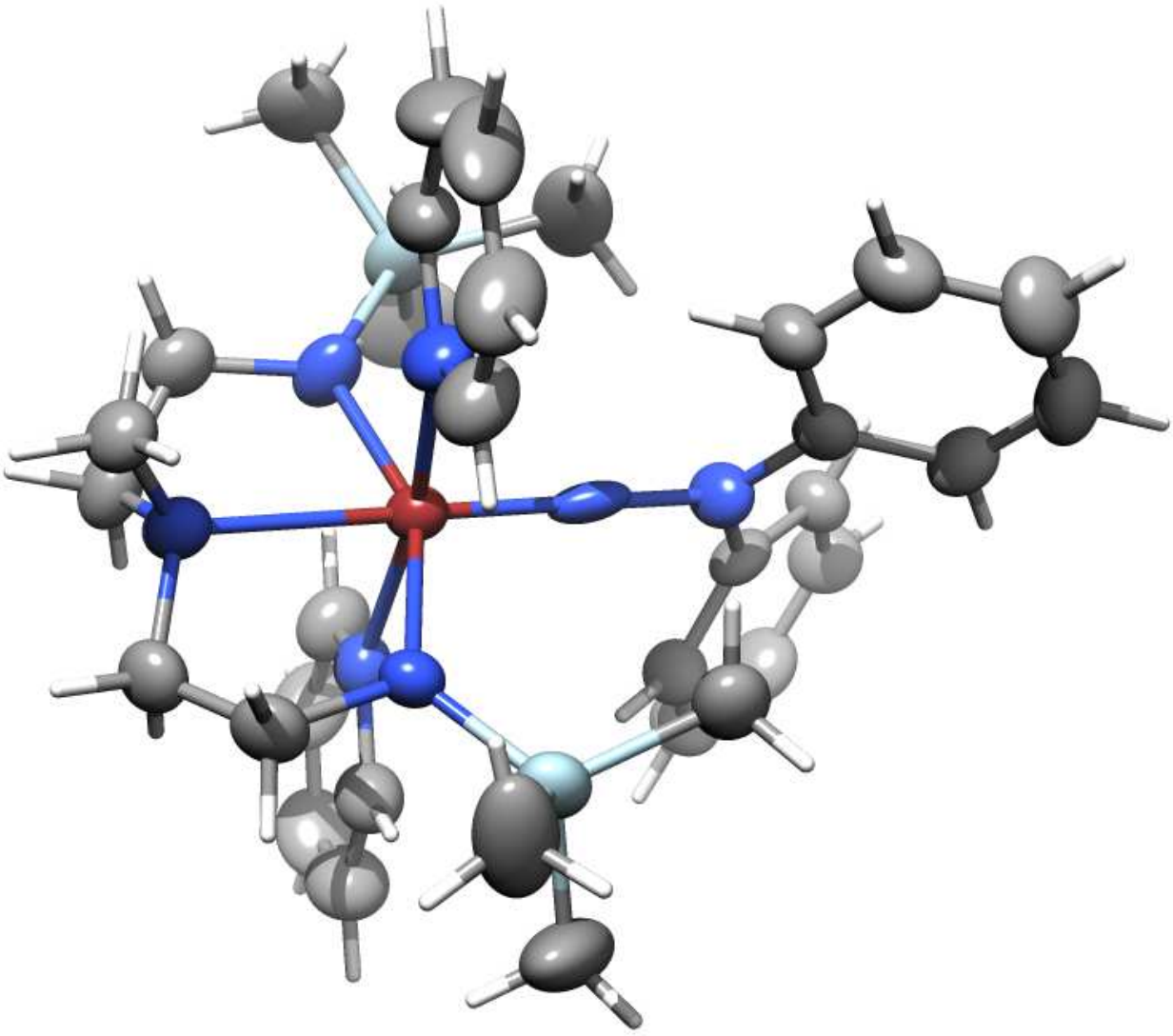
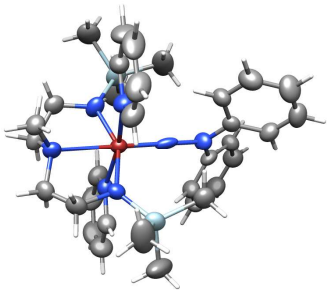
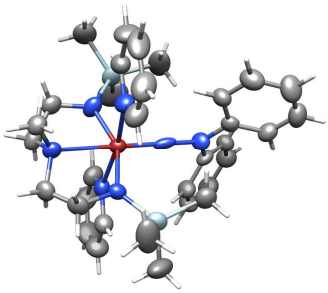
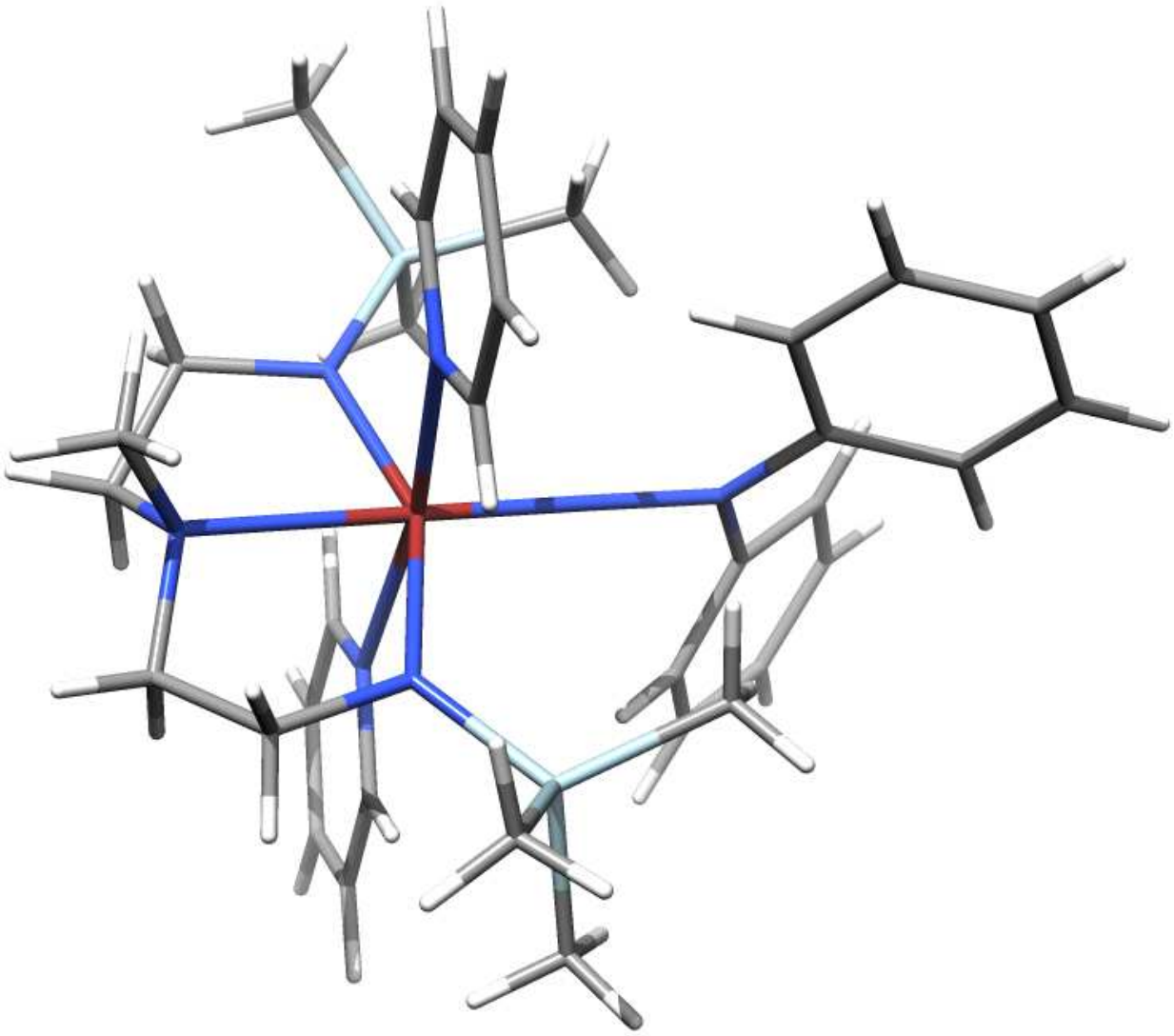
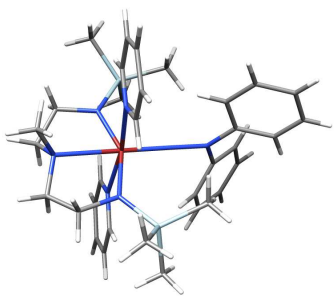
C14
C15











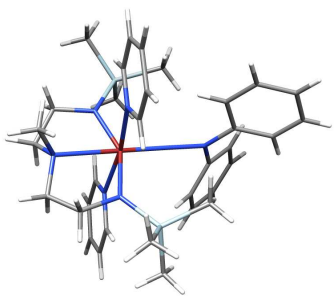


Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT37 (CCDC 739782). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	9309(1)	1855(1)	6894(1)	17(1)
Si(1)	8499(1)	3715(1)	5929(1)	29(1)
Si(2)	10191(1)	585(1)	8204(1)	27(1)
N(1)	9149(2)	612(2)	6181(1)	22(1)
N(2)	8814(2)	2531(2)	6084(1)	24(1)
N(3)	9794(2)	710(2)	7415(1)	19(1)
N(4)	10284(2)	2148(2)	6782(1)	21(1)
N(5)	8338(2)	1343(2)	6916(1)	25(1)
N(6)	9434(1)	2783(2)	7418(1)	19(1)
N(7)	9548(2)	3543(2)	7824(1)	22(1)
C(1)	8523(2)	44(2)	5995(2)	25(1)
C(2)	9150(2)	1116(2)	5650(2)	28(1)
C(3)	8703(2)	1996(2)	5523(2)	25(1)
C(4)	9723(2)	-28(2)	6465(2)	26(1)
C(5)	9831(2)	-209(2)	7112(2)	26(1)
C(6)	7715(2)	3703(3)	5227(2)	39(1)
C(7)	9092(2)	4564(3)	5812(2)	51(2)
C(8)	8300(2)	4233(3)	6537(2)	48(1)
C(9)	10008(3)	-635(3)	8407(2)	50(1)
C(10)	11112(2)	667(4)	8495(2)	54(2)
C(11)	9950(2)	1503(2)	8620(2)	31(1)
C(12)	10312(2)	2818(3)	6394(2)	29(1)
C(13)	10894(2)	3054(3)	6339(2)	35(1)
C(14)	11471(2)	2599(3)	6688(2)	38(1)
C(15)	11456(2)	1923(3)	7093(2)	34(1)
C(16)	10861(2)	1716(3)	7126(2)	26(1)
C(17)	7746(2)	1717(3)	6558(2)	29(1)
C(18)	7155(2)	1462(3)	6587(2)	41(1)
C(19)	7159(2)	777(3)	6993(2)	43(1)
C(20)	7758(2)	387(3)	7368(2)	38(1)
C(21)	8334(2)	680(3)	7321(2)	31(1)
C(22)	10077(2)	4172(2)	7875(2)	21(1)
C(23)	10647(2)	3794(3)	7846(2)	26(1)
C(24)	11146(2)	4395(3)	7848(2)	31(1)
C(25)	11093(2)	5383(3)	7898(2)	32(1)
C(26)	10532(2)	5750(3)	7946(2)	27(1)
C(27)	10023(2)	5162(2)	7928(2)	22(1)
C(28)	9165(2)	3615(2)	8163(2)	20(1)
C(29)	8558(2)	3143(3)	7976(2)	23(1)
C(30)	8193(2)	3166(3)	8318(2)	31(1)
C(31)	8426(2)	3666(3)	8852(2)	33(1)
C(32)	9024(2)	4141(3)	9038(2)	31(1)
C(33)	9394(2)	4125(2)	8705(2)	24(1)
B(1)	2648(2)	2484(3)	5315(2)	16(1)
F(1)	3113(1)	-1453(2)	4757(1)	82(1)
F(2)	3959(1)	-617(2)	5217(2)	70(1)
F(3)	3698(2)	-1709(2)	5651(1)	83(1)

F(4)	1788(2)	-1291(2)	6178(2)	97(1)
F(5)	1262(1)	6(2)	5983(1)	65(1)
F(6)	2130(1)	-96(2)	6765(1)	63(1)
F(7)	3601(3)	5550(2)	4569(2)	145(2)
F(8)	3321(2)	4690(3)	3830(2)	144(2)
F(9)	4306(1)	5023(2)	4309(1)	58(1)
F(10)	5597(1)	2481(2)	5563(2)	82(1)
F(11)	5050(1)	1223(2)	5515(1)	60(1)
F(12)	5326(1)	2096(2)	6266(1)	61(1)
F(13)	1525(1)	1817(1)	2927(1)	29(1)
F(14)	1602(1)	3349(2)	2929(1)	42(1)
F(15)	640(1)	2676(2)	2592(1)	36(1)
F(16)	-439(1)	2931(3)	3938(1)	81(1)
F(17)	130(1)	3455(2)	4800(1)	72(1)
F(18)	1(2)	1984(2)	4661(2)	104(1)
F(19)	4154(1)	2652(2)	7592(1)	38(1)
F(20)	3303(1)	2454(2)	7802(1)	41(1)
F(21)	3821(1)	3802(1)	7980(1)	26(1)
F(22)	2261(2)	6186(2)	6315(2)	77(1)
F(23)	1405(1)	5433(2)	5742(1)	70(1)
F(24)	1684(2)	5449(2)	6671(1)	71(1)
C(41)	2672(2)	1319(2)	5472(2)	14(1)
C(42)	3021(2)	645(2)	5296(2)	17(1)
C(43)	3027(2)	-331(2)	5428(2)	17(1)
C(44)	2650(2)	-669(2)	5717(2)	22(1)
C(45)	2271(2)	-24(3)	5871(2)	22(1)
C(46)	2294(2)	952(2)	5758(2)	20(1)
C(47)	3442(2)	-1008(2)	5258(2)	25(1)
C(48)	1866(2)	-362(3)	6194(2)	31(1)
C(49)	3297(2)	2825(2)	5202(2)	15(1)
C(50)	3274(2)	3623(2)	4840(2)	17(1)
C(51)	3824(2)	3925(2)	4748(2)	18(1)
C(52)	4423(2)	3447(2)	5007(2)	18(1)
C(53)	4471(2)	2677(2)	5381(2)	17(1)
C(54)	3922(2)	2394(2)	5482(2)	16(1)
C(55)	3763(2)	4791(3)	4364(2)	33(1)
C(56)	5110(2)	2139(3)	5678(2)	26(1)
C(57)	1939(2)	2618(2)	4724(2)	16(1)
C(58)	1879(2)	2606(2)	4134(2)	17(1)
C(59)	1263(2)	2658(2)	3643(2)	18(1)
C(60)	680(2)	2728(2)	3722(2)	21(1)
C(61)	722(2)	2724(2)	4302(2)	21(1)
C(62)	1335(2)	2664(2)	4787(2)	18(1)
C(63)	1253(2)	2629(3)	3025(2)	24(1)
C(64)	108(2)	2777(3)	4415(2)	36(1)
C(65)	2664(2)	3125(2)	5885(2)	16(1)
C(66)	3098(2)	2879(2)	6469(2)	15(1)
C(67)	3156(2)	3415(2)	6966(2)	17(1)
C(68)	2771(2)	4225(2)	6904(2)	19(1)
C(69)	2341(2)	4498(2)	6328(2)	19(1)
C(70)	2291(2)	3969(2)	5831(2)	18(1)
C(71)	3601(2)	3078(3)	7585(2)	22(1)
C(72)	1920(2)	5381(3)	6254(2)	31(1)

Table 3. Selected bond lengths [Å] and angles [°] for IAT37 (CCDC 739782).

Ta(1)-N(6)	1.762(3)	N(6)-Ta(1)-N(3)	103.59(12)
Ta(1)-N(3)	2.047(3)	N(6)-Ta(1)-N(2)	103.04(12)
Ta(1)-N(2)	2.055(3)	N(3)-Ta(1)-N(2)	153.07(12)
Ta(1)-N(5)	2.280(3)	N(6)-Ta(1)-N(5)	94.55(12)
Ta(1)-N(4)	2.314(3)	N(3)-Ta(1)-N(5)	89.82(12)
Ta(1)-N(1)	2.379(3)	N(2)-Ta(1)-N(5)	92.01(12)
		N(6)-Ta(1)-N(4)	94.70(12)
		N(3)-Ta(1)-N(4)	86.43(11)
		N(2)-Ta(1)-N(4)	87.49(12)
		N(5)-Ta(1)-N(4)	170.61(10)
		N(6)-Ta(1)-N(1)	179.25(13)
		N(3)-Ta(1)-N(1)	76.74(10)
		N(2)-Ta(1)-N(1)	76.59(11)
		N(5)-Ta(1)-N(1)	86.12(11)
		N(4)-Ta(1)-N(1)	84.64(10)

Table 4. Bond lengths [Å] and angles [°] for IAT37 (CCDC 739782).

Ta(1)-N(6)	1.762(3)	B(1)-C(41)	1.665(5)
Ta(1)-N(3)	2.047(3)	F(1)-C(47)	1.297(4)
Ta(1)-N(2)	2.055(3)	F(2)-C(47)	1.306(5)
Ta(1)-N(5)	2.280(3)	F(3)-C(47)	1.322(4)
Ta(1)-N(4)	2.314(3)	F(4)-C(48)	1.305(4)
Ta(1)-N(1)	2.379(3)	F(5)-C(48)	1.320(5)
Si(1)-N(2)	1.771(3)	F(6)-C(48)	1.325(5)
Si(1)-C(8)	1.862(5)	F(7)-C(55)	1.283(5)
Si(1)-C(6)	1.869(4)	F(8)-C(55)	1.276(5)
Si(1)-C(7)	1.871(5)	F(9)-C(55)	1.301(5)
Si(2)-N(3)	1.768(3)	F(10)-C(56)	1.307(5)
Si(2)-C(11)	1.844(4)	F(11)-C(56)	1.329(4)
Si(2)-C(10)	1.860(5)	F(12)-C(56)	1.319(5)
Si(2)-C(9)	1.862(4)	F(13)-C(63)	1.347(4)
N(1)-C(4)	1.469(4)	F(14)-C(63)	1.343(4)
N(1)-C(2)	1.477(5)	F(15)-C(63)	1.333(4)
N(1)-C(1)	1.492(4)	F(16)-C(64)	1.307(5)
N(2)-C(3)	1.490(4)	F(17)-C(64)	1.320(5)
N(3)-C(5)	1.500(4)	F(18)-C(64)	1.326(5)
N(4)-C(16)	1.345(5)	F(19)-C(71)	1.351(4)
N(4)-C(12)	1.351(5)	F(20)-C(71)	1.325(4)
N(5)-C(17)	1.343(5)	F(21)-C(71)	1.341(4)
N(5)-C(21)	1.357(5)	F(22)-C(72)	1.324(5)
N(6)-N(7)	1.402(4)	F(23)-C(72)	1.302(4)
N(7)-C(28)	1.408(5)	F(24)-C(72)	1.325(5)
N(7)-C(22)	1.424(5)	C(41)-C(46)	1.388(5)
C(2)-C(3)	1.524(5)	C(41)-C(42)	1.392(5)
C(4)-C(5)	1.521(5)	C(42)-C(43)	1.398(4)
C(12)-C(13)	1.386(6)	C(43)-C(44)	1.378(5)
C(13)-C(14)	1.362(6)	C(43)-C(47)	1.488(5)
C(14)-C(15)	1.378(6)	C(44)-C(45)	1.381(5)
C(15)-C(16)	1.378(6)	C(45)-C(46)	1.393(5)
C(17)-C(18)	1.383(6)	C(45)-C(48)	1.492(6)
C(18)-C(19)	1.374(6)	C(49)-C(54)	1.397(5)
C(19)-C(20)	1.374(6)	C(49)-C(50)	1.409(5)
C(20)-C(21)	1.382(6)	C(50)-C(51)	1.388(5)
C(22)-C(23)	1.392(5)	C(51)-C(52)	1.378(5)
C(22)-C(27)	1.396(5)	C(51)-C(55)	1.502(5)
C(23)-C(24)	1.383(5)	C(52)-C(53)	1.388(5)
C(24)-C(25)	1.393(5)	C(53)-C(54)	1.390(5)
C(25)-C(26)	1.387(6)	C(53)-C(56)	1.493(5)
C(26)-C(27)	1.377(5)	C(57)-C(58)	1.394(5)
C(28)-C(29)	1.391(5)	C(57)-C(62)	1.403(5)
C(28)-C(33)	1.403(5)	C(58)-C(59)	1.396(5)
C(29)-C(30)	1.379(5)	C(59)-C(60)	1.381(5)
C(30)-C(31)	1.380(5)	C(59)-C(63)	1.502(5)
C(31)-C(32)	1.376(5)	C(60)-C(61)	1.385(5)
C(32)-C(33)	1.370(6)	C(61)-C(62)	1.387(5)
B(1)-C(49)	1.639(6)	C(61)-C(64)	1.490(6)
B(1)-C(65)	1.644(5)	C(65)-C(66)	1.396(5)
B(1)-C(57)	1.645(5)	C(65)-C(70)	1.410(5)

C(66)-C(67)	1.386(5)	N(6)-N(7)-C(22)	115.4(3)
C(67)-C(68)	1.384(5)	C(28)-N(7)-C(22)	125.0(3)
C(67)-C(71)	1.503(5)	N(1)-C(2)-C(3)	109.0(3)
C(68)-C(69)	1.388(5)	N(2)-C(3)-C(2)	111.6(3)
C(69)-C(70)	1.387(5)	N(1)-C(4)-C(5)	109.2(3)
C(69)-C(72)	1.507(5)	N(3)-C(5)-C(4)	110.8(3)
		N(4)-C(12)-C(13)	123.0(4)
N(6)-Ta(1)-N(3)	103.59(12)	C(14)-C(13)-C(12)	119.5(4)
N(6)-Ta(1)-N(2)	103.04(12)	C(13)-C(14)-C(15)	118.4(4)
N(3)-Ta(1)-N(2)	153.07(12)	C(16)-C(15)-C(14)	119.4(4)
N(6)-Ta(1)-N(5)	94.55(12)	N(4)-C(16)-C(15)	123.3(4)
N(3)-Ta(1)-N(5)	89.82(12)	N(5)-C(17)-C(18)	123.4(4)
N(2)-Ta(1)-N(5)	92.01(12)	C(19)-C(18)-C(17)	119.4(4)
N(6)-Ta(1)-N(4)	94.70(12)	C(20)-C(19)-C(18)	118.3(4)
N(3)-Ta(1)-N(4)	86.43(11)	C(19)-C(20)-C(21)	119.5(4)
N(2)-Ta(1)-N(4)	87.49(12)	N(5)-C(21)-C(20)	123.0(4)
N(5)-Ta(1)-N(4)	170.61(10)	C(23)-C(22)-C(27)	119.5(4)
N(6)-Ta(1)-N(1)	179.25(13)	C(23)-C(22)-N(7)	119.2(3)
N(3)-Ta(1)-N(1)	76.74(10)	C(27)-C(22)-N(7)	121.2(4)
N(2)-Ta(1)-N(1)	76.59(11)	C(24)-C(23)-C(22)	120.4(4)
N(5)-Ta(1)-N(1)	86.12(11)	C(23)-C(24)-C(25)	120.2(4)
N(4)-Ta(1)-N(1)	84.64(10)	C(26)-C(25)-C(24)	118.9(4)
N(2)-Si(1)-C(8)	112.99(17)	C(27)-C(26)-C(25)	121.5(4)
N(2)-Si(1)-C(6)	108.76(16)	C(26)-C(27)-C(22)	119.5(4)
C(8)-Si(1)-C(6)	107.7(2)	C(29)-C(28)-C(33)	118.2(4)
N(2)-Si(1)-C(7)	112.67(19)	C(29)-C(28)-N(7)	120.2(3)
C(8)-Si(1)-C(7)	106.6(2)	C(33)-C(28)-N(7)	121.5(4)
C(6)-Si(1)-C(7)	107.9(2)	C(30)-C(29)-C(28)	120.9(4)
N(3)-Si(2)-C(11)	114.06(16)	C(29)-C(30)-C(31)	120.3(4)
N(3)-Si(2)-C(10)	112.61(19)	C(32)-C(31)-C(30)	119.2(4)
C(11)-Si(2)-C(10)	105.3(2)	C(33)-C(32)-C(31)	121.4(4)
N(3)-Si(2)-C(9)	108.49(17)	C(32)-C(33)-C(28)	120.0(4)
C(11)-Si(2)-C(9)	110.1(2)	C(49)-B(1)-C(65)	105.7(3)
C(10)-Si(2)-C(9)	106.0(2)	C(49)-B(1)-C(57)	113.6(3)
C(4)-N(1)-C(2)	113.1(3)	C(65)-B(1)-C(57)	111.4(3)
C(4)-N(1)-C(1)	109.3(3)	C(49)-B(1)-C(41)	112.0(3)
C(2)-N(1)-C(1)	108.8(3)	C(65)-B(1)-C(41)	110.3(3)
C(4)-N(1)-Ta(1)	104.9(2)	C(57)-B(1)-C(41)	104.0(3)
C(2)-N(1)-Ta(1)	104.2(2)	C(46)-C(41)-C(42)	115.6(3)
C(1)-N(1)-Ta(1)	116.7(2)	C(46)-C(41)-B(1)	120.5(3)
C(3)-N(2)-Si(1)	111.6(2)	C(42)-C(41)-B(1)	123.8(3)
C(3)-N(2)-Ta(1)	118.6(2)	C(41)-C(42)-C(43)	122.6(4)
Si(1)-N(2)-Ta(1)	129.82(17)	C(44)-C(43)-C(42)	120.1(4)
C(5)-N(3)-Si(2)	110.6(2)	C(44)-C(43)-C(47)	119.8(3)
C(5)-N(3)-Ta(1)	118.6(2)	C(42)-C(43)-C(47)	120.1(3)
Si(2)-N(3)-Ta(1)	130.77(15)	C(43)-C(44)-C(45)	118.6(3)
C(16)-N(4)-C(12)	116.4(4)	C(44)-C(45)-C(46)	120.4(4)
C(16)-N(4)-Ta(1)	122.3(3)	C(44)-C(45)-C(48)	120.0(3)
C(12)-N(4)-Ta(1)	121.2(3)	C(46)-C(45)-C(48)	119.5(4)
C(17)-N(5)-C(21)	116.4(4)	C(41)-C(46)-C(45)	122.6(4)
C(17)-N(5)-Ta(1)	122.2(3)	F(1)-C(47)-F(2)	107.0(4)
C(21)-N(5)-Ta(1)	121.3(3)	F(1)-C(47)-F(3)	103.9(3)
N(7)-N(6)-Ta(1)	177.6(3)	F(2)-C(47)-F(3)	103.9(4)
N(6)-N(7)-C(28)	119.6(3)	F(1)-C(47)-C(43)	113.4(3)

F(2)-C(47)-C(43)	114.5(3)	C(60)-C(61)-C(62)	120.4(4)
F(3)-C(47)-C(43)	113.2(4)	C(60)-C(61)-C(64)	120.5(4)
F(4)-C(48)-F(5)	105.9(4)	C(62)-C(61)-C(64)	119.1(4)
F(4)-C(48)-F(6)	107.8(4)	C(61)-C(62)-C(57)	123.1(4)
F(5)-C(48)-F(6)	103.8(4)	F(15)-C(63)-F(14)	106.9(3)
F(4)-C(48)-C(45)	113.5(4)	F(15)-C(63)-F(13)	106.2(3)
F(5)-C(48)-C(45)	113.5(3)	F(14)-C(63)-F(13)	105.5(3)
F(6)-C(48)-C(45)	111.7(4)	F(15)-C(63)-C(59)	112.8(3)
C(54)-C(49)-C(50)	115.0(3)	F(14)-C(63)-C(59)	112.5(3)
C(54)-C(49)-B(1)	123.2(3)	F(13)-C(63)-C(59)	112.3(3)
C(50)-C(49)-B(1)	121.8(3)	F(16)-C(64)-F(17)	105.6(4)
C(51)-C(50)-C(49)	122.1(3)	F(16)-C(64)-F(18)	105.7(4)
C(52)-C(51)-C(50)	121.2(3)	F(17)-C(64)-F(18)	103.6(4)
C(52)-C(51)-C(55)	119.8(4)	F(16)-C(64)-C(61)	114.7(4)
C(50)-C(51)-C(55)	119.0(3)	F(17)-C(64)-C(61)	113.4(3)
C(51)-C(52)-C(53)	118.3(4)	F(18)-C(64)-C(61)	112.8(4)
C(52)-C(53)-C(54)	120.1(3)	C(66)-C(65)-C(70)	115.4(3)
C(52)-C(53)-C(56)	120.6(3)	C(66)-C(65)-B(1)	120.0(3)
C(54)-C(53)-C(56)	119.3(3)	C(70)-C(65)-B(1)	124.5(3)
C(53)-C(54)-C(49)	123.2(3)	C(67)-C(66)-C(65)	122.7(3)
F(8)-C(55)-F(7)	105.7(4)	C(68)-C(67)-C(66)	120.9(3)
F(8)-C(55)-F(9)	105.7(4)	C(68)-C(67)-C(71)	118.9(3)
F(7)-C(55)-F(9)	104.6(4)	C(66)-C(67)-C(71)	120.1(3)
F(8)-C(55)-C(51)	112.7(3)	C(67)-C(68)-C(69)	117.9(3)
F(7)-C(55)-C(51)	112.8(4)	C(70)-C(69)-C(68)	121.2(3)
F(9)-C(55)-C(51)	114.6(4)	C(70)-C(69)-C(72)	120.5(3)
F(10)-C(56)-F(12)	106.9(4)	C(68)-C(69)-C(72)	118.4(3)
F(10)-C(56)-F(11)	105.9(4)	C(69)-C(70)-C(65)	121.9(3)
F(12)-C(56)-F(11)	103.3(3)	F(20)-C(71)-F(21)	107.4(3)
F(10)-C(56)-C(53)	114.1(3)	F(20)-C(71)-F(19)	107.5(3)
F(12)-C(56)-C(53)	113.4(3)	F(21)-C(71)-F(19)	105.4(3)
F(11)-C(56)-C(53)	112.4(3)	F(20)-C(71)-C(67)	112.4(3)
C(58)-C(57)-C(62)	115.0(3)	F(21)-C(71)-C(67)	112.6(3)
C(58)-C(57)-B(1)	124.0(3)	F(19)-C(71)-C(67)	111.2(3)
C(62)-C(57)-B(1)	120.8(3)	F(23)-C(72)-F(22)	106.9(3)
C(57)-C(58)-C(59)	122.3(4)	F(23)-C(72)-F(24)	105.8(4)
C(60)-C(59)-C(58)	121.1(4)	F(22)-C(72)-F(24)	103.8(3)
C(60)-C(59)-C(63)	120.9(3)	F(23)-C(72)-C(69)	114.2(3)
C(58)-C(59)-C(63)	118.0(4)	F(22)-C(72)-C(69)	112.7(4)
C(59)-C(60)-C(61)	118.0(3)	F(24)-C(72)-C(69)	112.6(3)

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT37 (CCDC 739782). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	157(1)	137(1)	199(1)	-4(1)	46(1)	-4(1)
Si(1)	344(8)	187(6)	252(6)	25(5)	30(5)	43(5)
Si(2)	295(8)	246(6)	235(6)	37(5)	75(5)	96(5)
N(1)	220(20)	164(15)	225(18)	2(13)	35(15)	20(15)
N(2)	290(20)	160(16)	211(18)	11(13)	34(15)	-25(15)
N(3)	174(19)	172(15)	214(17)	0(13)	68(14)	23(14)
N(4)	210(20)	182(16)	207(17)	-41(13)	67(15)	-23(14)
N(5)	180(20)	242(17)	274(19)	-70(15)	42(15)	-38(15)
N(6)	92(18)	181(15)	226(17)	97(13)	0(13)	-9(13)
N(7)	200(20)	159(15)	272(19)	-59(14)	71(15)	-40(14)
C(1)	230(30)	200(20)	270(20)	-41(17)	61(18)	-38(18)
C(2)	330(30)	240(20)	230(20)	-50(17)	66(19)	-42(19)
C(3)	260(20)	230(20)	230(20)	16(17)	60(17)	-5(18)
C(4)	280(30)	172(19)	300(20)	-40(17)	91(19)	14(18)
C(5)	280(30)	177(19)	300(20)	23(17)	87(19)	59(18)
C(6)	410(30)	300(20)	370(30)	50(20)	60(20)	150(20)
C(7)	560(40)	170(20)	630(30)	160(20)	90(30)	10(20)
C(8)	640(40)	270(20)	370(30)	-10(20)	60(20)	250(20)
C(9)	900(40)	280(20)	300(30)	70(20)	230(30)	160(30)
C(10)	330(30)	900(40)	290(30)	-30(30)	10(20)	220(30)
C(11)	350(30)	280(20)	240(20)	22(17)	70(20)	79(19)
C(12)	300(30)	290(20)	260(20)	1(18)	84(19)	-40(19)
C(13)	320(30)	410(20)	350(20)	-40(20)	160(20)	-170(20)
C(14)	290(30)	400(30)	500(30)	-110(20)	240(20)	-150(20)
C(15)	250(30)	340(20)	430(30)	-40(20)	130(20)	-30(20)
C(16)	240(30)	240(20)	290(20)	-44(17)	100(19)	-30(19)
C(17)	210(30)	310(20)	320(20)	-105(18)	74(19)	-10(20)
C(18)	160(30)	540(30)	470(30)	-130(20)	70(20)	-40(20)
C(19)	300(30)	630(30)	470(30)	-260(30)	260(20)	-230(30)
C(20)	360(30)	440(30)	370(30)	-80(20)	180(20)	-180(20)
C(21)	290(30)	320(20)	300(20)	-37(19)	90(20)	-90(20)
C(22)	140(20)	250(20)	180(20)	-32(16)	15(16)	-42(18)
C(23)	210(30)	250(20)	280(20)	-85(17)	67(18)	-33(19)
C(24)	170(30)	350(20)	380(30)	-121(19)	103(19)	-40(20)
C(25)	270(30)	290(20)	340(30)	-74(18)	80(20)	-110(20)
C(26)	280(30)	190(20)	330(30)	-2(17)	110(20)	-45(19)
C(27)	210(20)	180(19)	270(20)	-32(16)	98(18)	-8(18)
C(28)	200(20)	163(18)	220(20)	1(16)	62(17)	37(17)
C(29)	200(20)	221(18)	280(20)	-57(18)	100(17)	0(20)
C(30)	240(30)	270(20)	420(30)	-50(20)	150(20)	-30(20)
C(31)	420(30)	310(20)	340(30)	-20(20)	240(20)	-60(20)
C(32)	400(30)	300(20)	220(20)	-21(17)	120(20)	10(20)
C(33)	230(30)	220(20)	230(20)	-21(16)	44(18)	-28(18)
B(1)	140(30)	140(20)	160(20)	5(16)	36(18)	14(18)
F(1)	361(19)	1150(20)	750(20)	-729(19)	12(16)	170(17)
F(2)	550(20)	316(14)	1540(30)	-136(17)	720(20)	-29(14)

F(3)	1350(30)	690(20)	710(20)	375(17)	670(20)	750(20)
F(4)	1780(40)	286(15)	1710(40)	-112(18)	1590(30)	-243(19)
F(5)	357(19)	1020(20)	660(20)	275(17)	289(15)	-58(17)
F(6)	600(20)	1080(20)	284(16)	-30(15)	255(14)	-312(18)
F(7)	2900(60)	363(18)	2380(50)	700(20)	2390(50)	720(30)
F(8)	1080(30)	1440(30)	890(30)	950(30)	-510(20)	-850(30)
F(9)	402(19)	488(16)	960(20)	408(15)	394(17)	75(14)
F(10)	235(18)	870(20)	1420(30)	740(20)	422(19)	252(16)
F(11)	402(18)	397(15)	750(20)	-134(14)	-10(15)	194(13)
F(12)	464(19)	900(20)	312(16)	2(14)	-13(13)	382(16)
F(13)	328(14)	300(11)	239(12)	-21(10)	110(10)	62(11)
F(14)	617(19)	369(14)	287(14)	-6(10)	209(13)	-207(13)
F(15)	294(16)	494(14)	180(12)	6(10)	-28(11)	104(12)
F(16)	158(16)	1830(30)	343(16)	-184(19)	15(12)	155(19)
F(17)	296(18)	1240(30)	650(20)	-504(19)	237(15)	-104(16)
F(18)	650(30)	880(20)	1980(40)	490(30)	950(30)	120(20)
F(19)	326(16)	472(14)	227(13)	-56(11)	-12(11)	224(12)
F(20)	452(18)	401(13)	249(13)	121(11)	22(12)	-142(13)
F(21)	237(14)	316(12)	186(12)	-76(9)	40(10)	-8(10)
F(22)	570(20)	207(14)	1530(30)	10(16)	430(20)	90(14)
F(23)	610(20)	647(18)	507(19)	-171(14)	-127(15)	480(16)
F(24)	1020(30)	669(19)	690(20)	206(16)	600(20)	585(18)
C(41)	80(20)	182(18)	107(19)	8(14)	-29(15)	-6(16)
C(42)	160(20)	189(19)	130(19)	-6(15)	31(16)	-18(17)
C(43)	130(20)	152(18)	180(20)	-31(15)	16(16)	-28(16)
C(44)	250(30)	137(18)	210(20)	-7(15)	30(18)	-52(18)
C(45)	240(30)	250(20)	170(20)	5(16)	76(17)	-72(18)
C(46)	180(20)	190(19)	200(20)	-48(15)	58(17)	-24(17)
C(47)	270(30)	164(19)	320(20)	-12(17)	110(20)	-45(19)
C(48)	390(30)	240(20)	340(30)	7(19)	190(20)	-10(20)
C(49)	130(20)	150(17)	147(19)	-54(14)	45(16)	-24(15)
C(50)	140(20)	154(18)	180(20)	-34(15)	20(16)	-1(16)
C(51)	170(20)	160(18)	180(20)	-34(15)	35(16)	-42(17)
C(52)	130(20)	210(19)	210(20)	-43(15)	64(16)	-61(16)
C(53)	110(20)	175(18)	200(20)	-49(16)	33(16)	-18(16)
C(54)	190(20)	137(18)	136(19)	-40(14)	35(16)	-18(16)
C(55)	280(30)	280(20)	400(30)	100(20)	100(20)	-40(20)
C(56)	160(30)	250(20)	360(30)	13(18)	86(19)	-8(18)
C(57)	170(20)	85(17)	180(20)	-20(14)	46(17)	-46(16)
C(58)	140(20)	100(17)	240(20)	-11(15)	57(17)	-12(16)
C(59)	200(20)	98(17)	170(20)	-1(15)	19(17)	0(17)
C(60)	180(20)	152(18)	190(20)	9(15)	-36(17)	8(17)
C(61)	130(20)	174(18)	280(20)	-39(16)	41(17)	-15(17)
C(62)	170(20)	158(18)	190(20)	-16(15)	47(17)	-30(17)
C(63)	210(30)	240(20)	220(20)	35(17)	33(18)	1(19)
C(64)	220(30)	460(30)	340(30)	-60(20)	70(20)	-30(20)
C(65)	110(20)	150(16)	202(19)	-8(16)	60(15)	-30(17)
C(66)	110(20)	121(18)	220(20)	-19(14)	64(16)	-3(15)
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C(69)	150(20)	170(18)	250(20)	-6(16)	85(17)	0(16)
C(70)	170(20)	170(18)	180(20)	5(15)	40(17)	-27(17)
C(71)	190(20)	230(19)	230(20)	-25(18)	63(17)	0(20)
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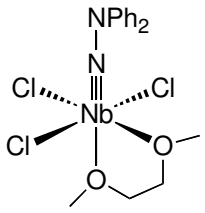
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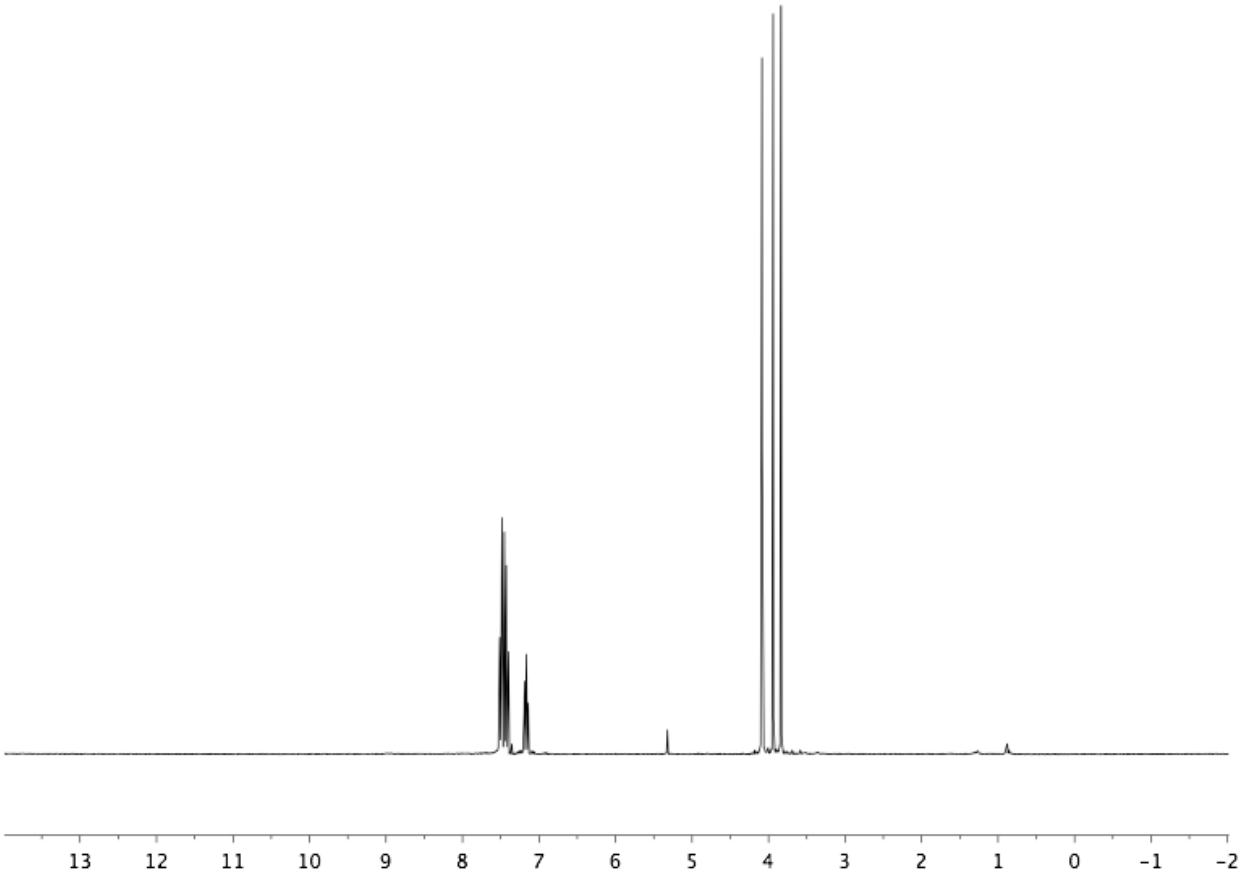
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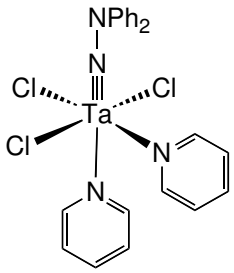
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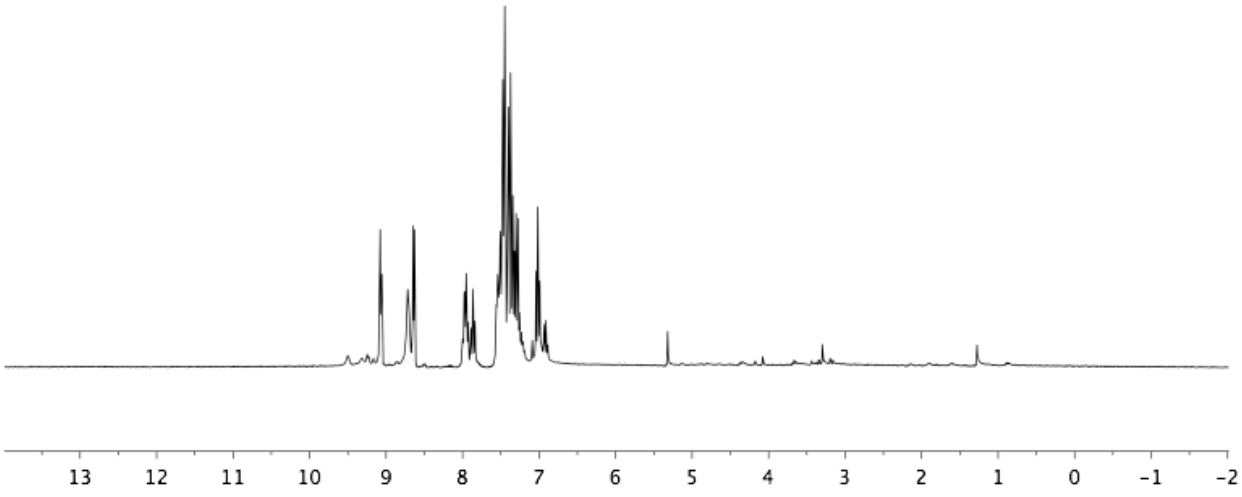
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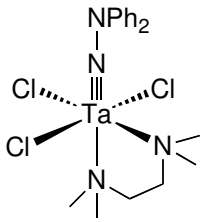
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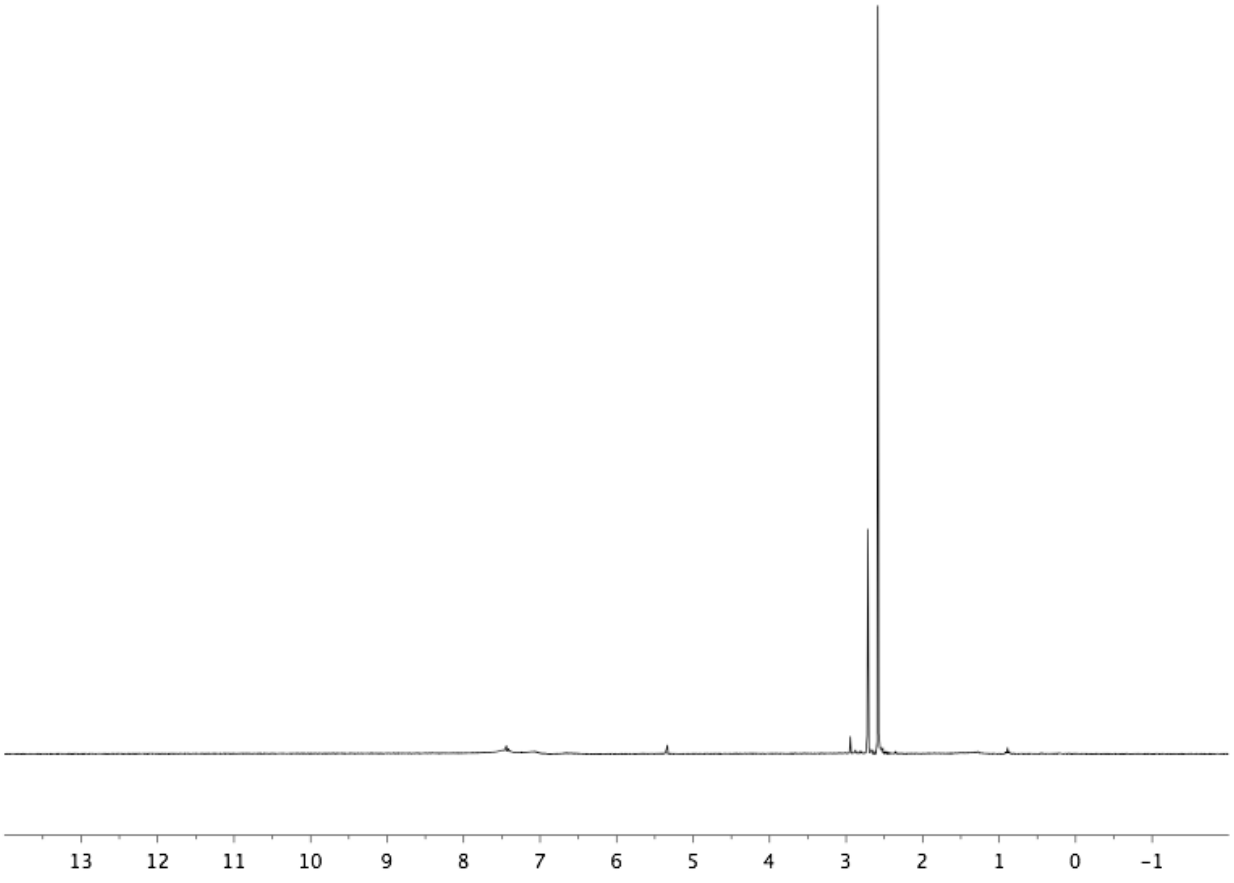
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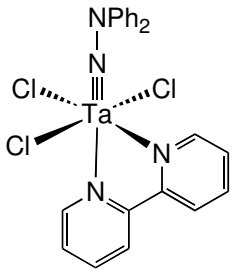
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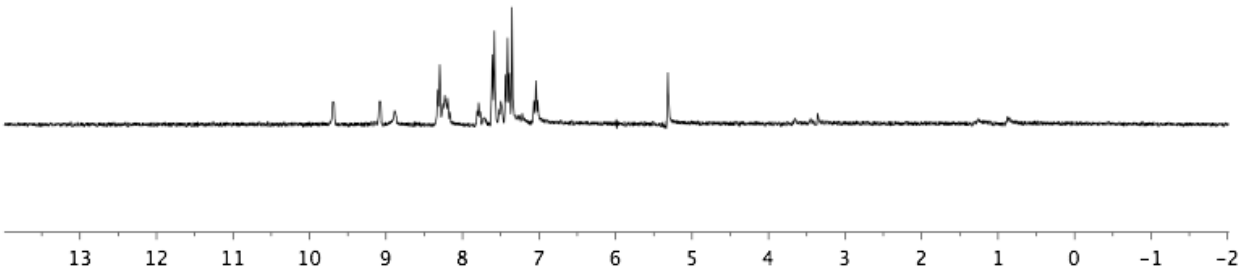
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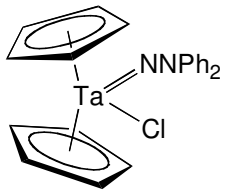
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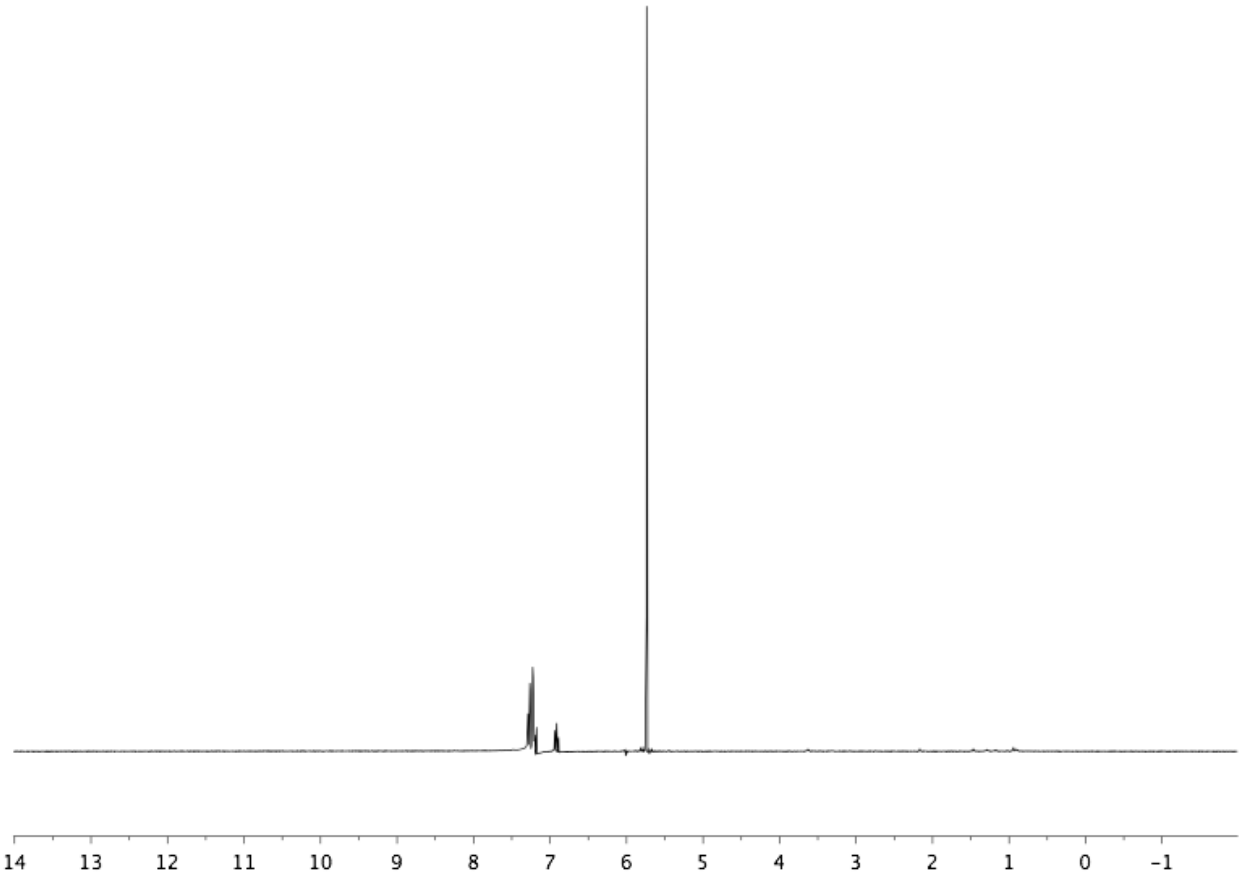
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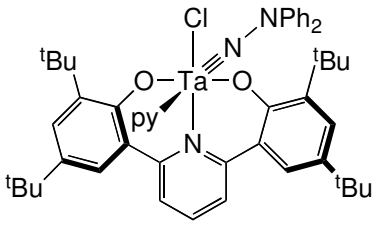
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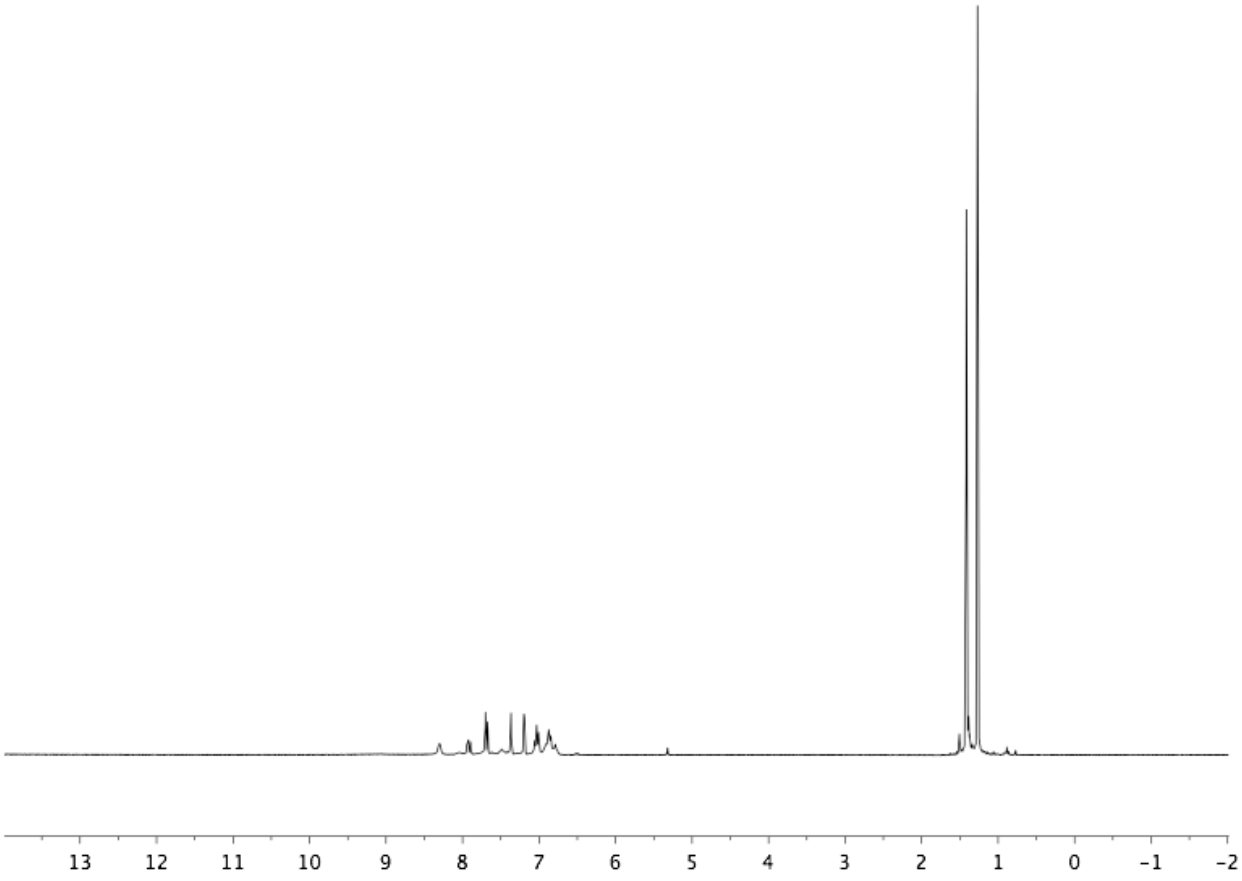
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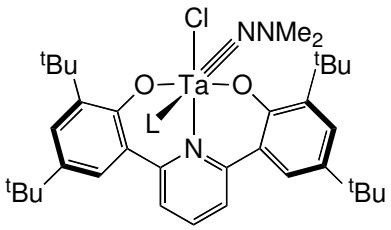

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